LBID-2440

Proposals for Yucca Mountain Science and Technology Program

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Earth Sciences Division

Ardyth M. Simmons, Editor

Preface

The U.S. Department of Energy's Director of the Office Civilian Radioactive Waste Management (OCRWM), Dr. Margaret Chu, has mandated the establishment of a continuing science and technology (S&T) program. As she stated to the Nuclear Waste Technical Review Board on September 10, 2002, the planned sustained S&T program must be committed to the following:

- Increasing confidence in repository performance by reducing uncertainty
- Enhancing efficiencies and reducing life-cycle costs
- Improving existing technologies and developing new ones
- Maintaining U.S. leadership in nuclear waste management.

The S&T program may also enhance confidence during review of the License Application, such that relevant information will be integrated into licensing-related activities. Other activities could be implemented in the longer term through the Performance Confirmation program.

The proposals contained herein are an outgrowth of Dr. Margaret Chu's mandate to establish a continuing S&T program. This report contains 16 proposals and their overview that were presented to Mr. Stephan Brocoum and Mr. Dennis Williams of the OCRWM Yucca Mountain Project on August 15, 2002. Each investigation has two overriding purposes in advancing the OCRWM program: (1) to lead to reduction of life-cycle costs, and (2) to reduce uncertainty, and thereby reduce risk, by enhancing the contribution of the natural system to system performance. The work proposed is new science. For example, one proposal could reduce risk by quantifying the thermal-hydrological-mechanical processes that would come into play when a volcanic dike intercepts a waste disposal drift. Another proposal provides for life-cycle cost-saving measures by reducing ventilation costs through a value-based option approach to purchasing electricity. A third proposal provides for significant improvement in performance of the natural barrier through quantifying the efficacy of the drift shadow zone beneath YM drifts, and by extending confidence through study of drift shadow analogues. Other proposals deal with improved understanding of flow – fast flow, capillary barriers, fracture flow, film flow – and transport – by colloids, nano-particles, in intact rock and along fractures, faults and features under unsaturated conditions. These examples are only a sampling of the many areas in which uncertainty can be reduced; other examples in the proposals include improved gridding in numerical models, fully coupled climate models for greenhouse gas effects, and an enhanced understanding of scaling. A listing of all the proposals, their potential benefits, and anticipated cost reduction is shown in Table Pr-1*. A schematic cross-section (Figure Pr-1) shows how individual proposals relate to various aspects or components of the natural and engineered barriers at the proposed Yucca Mountain repository.

Each proposal focuses on a specific heretofore unsolved problem and the impact to the Yucca Mountain Project of not solving the problem. This is followed by a description of proposed workscope, schedule, and estimated resources needed to complete the work. The multi-faceted problem-solving approaches in these proposals include laboratory and field investigations coupled to numerical modeling. When possible, results of studies plan for reality checking against multiple lines of evidence, particularly natural analogues. Discrete natural analogue studies are also proposed in areas that contribute to confidence-building of process models within the natural barrier system. Many of the proposals involve collaboration with universities, national laboratories, and other research institutions in the U.S. as well as with international programs.

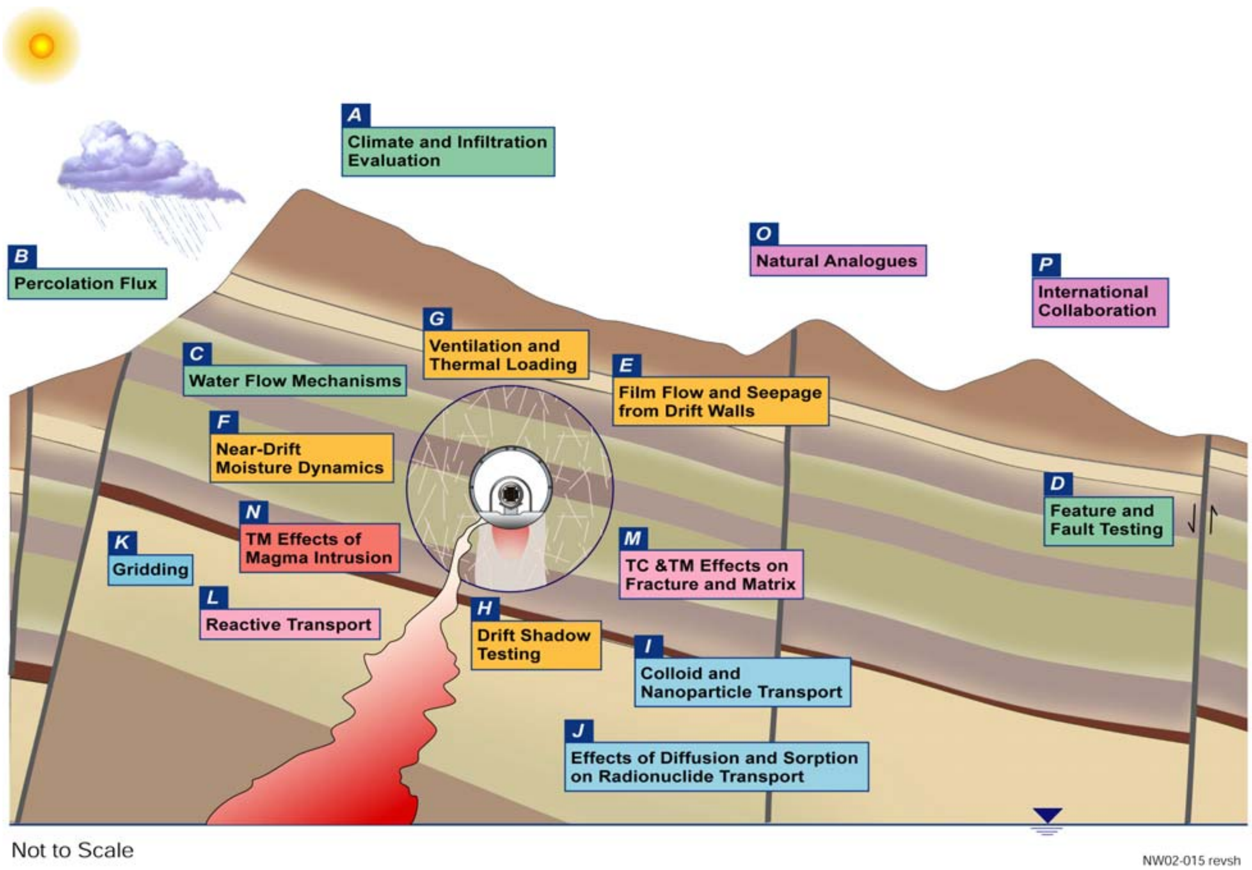
Questions regarding the technical content of individual proposals may be directed to the contact individual named on the proposal or to Earth Sciences Division Director, Bo Bodvarsson, at (510) 486-4789 (gsbodvarsson@lbl.gov). Questions about this LBNL report itself may be directed to me at (510) 486-7106 (amsimmons@lbl.gov).

Ardyth M. Simmons
November 19, 2002

* The cost reduction can be expressed in terms of *direct* savings, high or moderate savings for *basic* understanding or *improvement* of natural barrier performance, or *potential* savings worthy of investment.

Table Pr 1 - Benefits and Potential Cost Reduction of Proposals

	Title	Benefit	Cost Reduction to Program
A	Climate and Infiltration Evaluation	Reduces uncertainty through a realistic climate model, including greenhouse gas effects	Moderate Improvement
B	Percolation Flux	Reduces uncertainty in percolation flux, improves confidence in UZ models	High Basic
C	Water Flow Mechanisms in the Unsaturated Zone	Reduces uncertainty in flow abstraction in UZ models	Moderate Basic
D	Feature and Fault Testing and Analysis	Reduces uncertainty in role of faults and features as flow paths	Moderate Improvement
E	Film Flow and Seepage From Drift Walls	Reduces uncertainty in relative roles of dripping and film flow, may reduce waste package corrosion	High Basic
F	Near-Drift Moisture Dynamics	Increases confidence needed for ventilation model	High Basic
G	Ventilation System for Thermal Load Control	Provides decision-making framework for design and operation of ventilation system	Very high Direct
H	Drift Shadow Testing	Increases confidence in natural barrier transport pathways	High Basic
I	Colloid and Nanoparticle Transport in the Unsaturated Zone	Increases confidence in role of colloids and nanoparticles for transport models	High Basic
J	Effects of Diffusion and Sorption on Radionuclide Transport in the Unsaturated Zone	Reduces uncertainty by providing more realistic assessment of sorption and diffusion	Moderate Improvement
K	Improved Spatial Discretization Techniques	Reduces risk by increasing confidence in model accuracy	Potential
L	Reactive-Transport Parameters and Processes in the Unsaturated Zone	Reduces uncertainty by increasing realism in reactive transport modeling	High Basic
M	Thermal-Chemical and Thermal-Mechanical Effects on Fracture and Matrix Properties	Reduces uncertainty about fracture sealing	Moderate Improvement
N	Multiscale Thermomechanical Effects of Magma Intrusion on Drifts and the Unsaturated Zone	Reduces uncertainty and risk regarding magma intrusion into drifts	Potential
O	Building Confidence through Natural Analogues	Provides qualitative model validation and increased public confidence	Moderate Improvement
P	Building Confidence through International Collaboration	Potential for development of new approaches, insights, increased scientific confidence	Potential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O
Natural Analogues
P
International Collaboration
Not to Scale
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A. Climate and Infiltration Evaluation with Global to Site-Scale Nested Modeling

Focus Area: Climate, Unsaturated Zone
Contact: Norman L. Miller, NLMiller@lbl.gov, (510) 495-2374
Collaboration: LBNL and National Energy Research Scientific Computing Center

Statement of Problem

Understanding future climate and unsaturated zone impacts at Yucca Mountain requires process-based simulations using a fully coupled atmosphere-land surface-subsurface model with space and time dependent feedback. Such a physically based approach should include an analysis of the physical and dynamical response to anthropogenic Green House Gas (GHG)-related climate changes. Three questions are posed to reduce uncertainties in the analysis of future climate and unsaturated zone infiltration: (1) What climatic mechanisms, including effects due to increased atmospheric carbon dioxide concentrations (i.e. GHG), can cause an infiltration threshold exceedence, (infiltration threshold is defined here as the infiltration rate at which a radionuclide plume beneath the repository advects and can reach the groundwater within a time period to be determined), and what is the likelihood of exceeding such a threshold? (2) How can spatio-temporal recharge and discharge distribution in the unsaturated zone at Yucca Mountain be physically determined, and what are the appropriate scales for evaluation? (3) How do the atmosphere, land surface, and subsurface processes interact with each other within the boundary zone, and how does this boundary zone act as the first natural barrier system for the potential repository?

Background

Present USGS estimates of net infiltration at Yucca Mountain are approximately 5 mm/year with mean-annual precipitation on order 100 mm/year. The future climate analysis (Forrester 2001) states that the modern-day climate should persist for 400 to 600 years, followed by a warmer and much wetter monsoon climate for 900 to 1400 years, followed by a cooler and wetter glacial-transition climate. The upper bound precipitation for the monsoon and glacial-transition climates exceeds the modern-day climate and the glacial-transition lower bound exceeds the modern lower bound values with a decreased evaporation rate. This future climate analysis is very conservative, used historical records and analogies to extrapolate future climatic precipitation rates, and is decoupled from atmosphere, land surface, and subsurface processes at Yucca Mountain. The suggested probabilities of atmospheric wetness (Forrester 2001) at Yucca Mountain remain very uncertain. A recent report by the Desert Research Institute suggests that the monsoon climate already began 1,000 years ago (Sharpe 2002, p. 52), further articulating the uncertainty and conservatism of the future climate analysis.

Previous infiltration studies at the Yucca Mountain site have assumed a one-dimensional steady-state model, and only evaluated mean-annual infiltration. Those approaches cannot answer the question of how a critical infiltration threshold could occur. Additionally, a mean-annual infiltration does not take into account the impacts associated with sub-annual intense precipitation events, persisting precipitation, and surface processes that may lead to overland flow and infiltration along a fault. Such steady-state annual-rate assumptions average out, or reduce, the potential impact of net infiltration as a transient phenomenon.

The dynamical and physical responses to GHG-related climate change have not been fully developed in the Yucca Mountain analysis (Forrester 2001). Recent observations and global climate simulations (IPCC 2000) have indicated a change in the frequency and strength of the El Niño Southern Oscillation (ENSO), a climatic mechanism that indicates above (positive-phase) and below (negative-phase) average precipitation in the southwestern U.S. Other oscillations that can superimpose on ENSO (e.g. North American Monsoon, Pacific Decadal Oscillation, etc.), and may impact at Yucca Mountain, have not been evaluated within the context of GHG-related climate change intense and persistent precipitation. Understanding downscaled climate and hydrology of the southwestern U.S. (Miller et al. 1999) using physically based climate models can reduce the uncertainties in estimating future climate.

Impact/Importance to the Yucca Mountain Project

The existing understanding of future climate at Yucca Mountain has a large uncertainty and is very conservative, based on records of analogue sites. By developing a fully coupled atmospheric-land surface-subsurface model specifically for Yucca Mountain, this uncertainty, as well as the uncertainty of the unsaturated zone infiltration, will be reduced. Implementation of a process-based land surface model with vegetation, and root zone physical descriptions coupled to an atmospheric model, with GHG-related climate changes taken into account, will better define unsaturated zone infiltration, its parameters, and the probabilities of wetter or drier future climates. It is likely that future climate analysis overestimates the precipitation during the modern monsoon climate. Such an advanced coupled regional climate system model will provide a more physically sound estimation of net infiltration, an ultimate driving force of all UZ processes. The net infiltration rate has been found to be the most significant factor that impacts unsaturated zone flow and radionuclide transport at Yucca Mountain (Wu et al. 2001).

Objective

Physically-based climate scenarios of present and future climate will be generated and mechanisms will be evaluated that may set up intense and/or persistent precipitation in conjunction with the development of a state-of-the-art fully coupled atmosphere-land surface-subsurface regional climate system model. This will provide a more accurate estimation of maximum, minimum, and mean infiltration, and will quantify a critical infiltration *threshold* and its likelihood of occurrence at the Yucca Mountain.

Workscope

1. Climatological Analysis

   - Obtain and/or generate, in collaboration with NERSC, global climate system model (NCAR CSM.2) simulations of historical (1950-2000) and future climates. Future climate simulations will include increases in atmospheric carbon dioxide concentration to more than four times present levels.
   - Analyze historical simulations of atmospheric dynamics and precipitation bias as compared with observations.
   - Analyze sensitivity of future climate as compared to historical simulations.

2. Model Development and Evaluation

   - Develop a fully coupled atmosphere-land surface-subsurface regional climate system model using state-of-art codes, including the NCAR Mesoscale Model version 5 (MM5) or NOAA/NCAR Weather Research and Forecast (WRF) model and TOUGH. (See Figure A-1)
   - Develop a methodology for coupling physically based atmosphere-land surface-subsurface processes and implement the methodology into a general numerical code that couples and models atmosphere, surface water, and groundwater systems with feedback.
   - Develop a grid system for passing fluxes across the land surface-subsurface model interface. This requires a grid matching technique that conserves mass and energy across the interface.
   - Develop a surface (boundary zone) physical/chemical reaction model to couple atmosphere, surface and groundwater interactions on the land surface, including water and energy exchanges.
   - Evaluate infiltration and time-evolving soil moisture with the neutron-moisture probe data and the observed stream flow data.
   - Evaluate the NCAR CSM.2 simulated historical climate using the NCAR/NCEP Reanalysis and NASA Land Data Assimilation System (LDAS), as available.

3. Fully Coupled Model Studies of Infiltration Threshold

   - Perturb historical and future climate simulations until an infiltration threshold is exceeded. This is accomplished by applying the climate signal as input to a coupled land surface-subsurface model via statistical downscaling and increasing the precipitation until an infiltration rate above 200 mm/year and other short-term infiltration rates (to be determined) are reached. An infiltration of rate of 200 mm/yr was suggested as a critical threshold value for Yucca Mountain (G. Bodvarsson, personal communication).
   - Dynamically downscale NCAR CSM.2 future climate and perturbed simulations using the newly developed and evaluated coupled regional climate system model to the site scale. This sensitivity study will evaluate increases in precipitation and water cycle dynamics as the Yucca Mountain site

infiltration threshold is reached. It is expected that a number of mechanisms cause this to occur. Each will be further evaluated for likelihood of occurrence.

- Simulate infiltration through the boundary zone under current and future climate conditions with the fully coupled regional climate system model, providing more accurate, physically based, spatio-temporal distributions of infiltration water (the upper boundary of UZ).

Schedule

Year 1:

- Develop land surface-subsurface coupling procedure, test, and evaluate.
- Test the regional atmospheric model (WRF or MM5) with the state-of-art land surface model for the southwestern U.S. and Yucca Mountain. This is a double-nested procedure where output from the large WRF (or MM5) southwestern U.S. regional domain is used as input forcing for the WRF (or MM5) fine-scale Yucca Mountain Site domain
- Evaluate historical NCAR CSM.2 climate simulation (e.g. 1950 – 2000)

Year 2:

- Analyze results of CSM.2 historical run and the land surface-subsurface model interface
- Develop the coupled atmosphere-land surface-subsurface system model
- Begin test runs and analysis with the coupled system model
- Perform ensemble simulations of future climate projections using the NCAR CSM.2, which include a transient one-percent annual increase of atmospheric carbon dioxide concentration
- Perform perturbed simulations using CSM.2 and statistical downscaling until an infiltration threshold is reached.

Year 3:

- Continue system model evaluation and testing.
- Perform dynamic downscaling using to-be-specified perturbed CSM2 simulations with the coupled WRF-TOUGH system model
- Develop new estimates of the range of infiltration and the uncertainty.

Products

- An evaluated coupled regional climate system model with current state-of-art atmosphere, land surface, and subsurface descriptions.
- Annual Progress Reports.
- Peer reviewed journal articles: (1) atmosphere-land surface-surface regional climate system model coupling and evaluation, (2) global climate control and projected simulations and analysis, (3) probabilities of an infiltration threshold exceedence at Yucca Mountain.
- Data sets: more accurately estimated net infiltration maps that can significantly reduce uncertainties in Total System Performance Assessment (TSPA) of the Yucca Mountain site.

Level of Effort

Personnel: 3.25 FTEs/yr (36 person-months per year for three years; NERSC computer time = 0.25)

Equipment: 3 state-of-the-art multi-processor Linux Work Stations (~$5K each), 500GB storage (~$5K).

Travel: 2 science conferences/year/investigator, Yucca Mountain coordinating meetings

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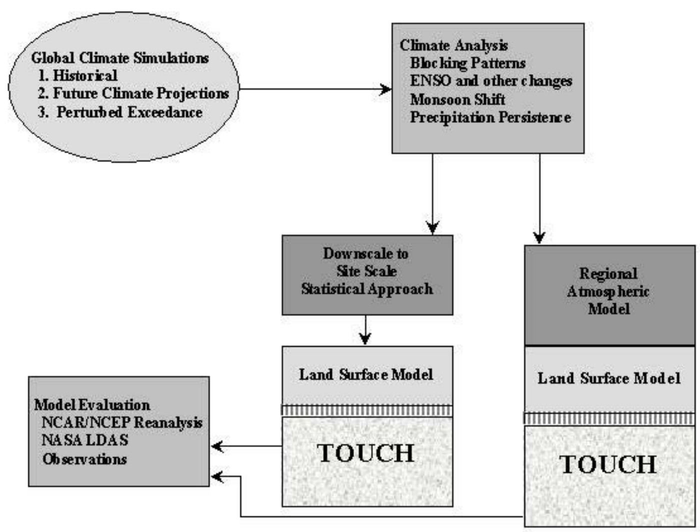

Figure A-1. Schematic of research approach

B. Application of Geochemical Data to Bound Current and Past Infiltration Rates

Focus Area: Unsaturated Zone
Contact: Patrick Dobson, PFDobson@lbl.gov, (510) 486-5373
Collaboration: LBNL, USGS, LANL

Statement of Problem

Characterization of fluid flow and chemistry in fractured unsaturated rock at a variety of scales is critical in understanding and modeling fluid flow and transport. The presence of bomb-pulse tritium and ^{36}Cl in some areas within the Exploratory Studies Facility (ESF) at Yucca Mountain strongly suggests that relatively rapid flow (>300 m distance in less than 50 years) has occurred along certain flow paths (Figure B-1), (Fabryka-Martin et al. 1997). Fast-flow paths along fractures and faults are of great importance in assessing the long-term performance of a potential high-level radioactive waste repository at Yucca Mountain. However, chemical and isotopic characteristics of pore waters suggest that most of the water in the unsaturated zone (UZ) at Yucca Mountain travels at much slower rates. The identity of the fast-flow paths and their significance to overall fluid flow and transport within the UZ at Yucca Mountain are not well understood.

Field tensiometry measurements at Yucca Mountain are all around 1 bar, suggesting minimal variation of water potential throughout the UZ. The presence of nearly uniform water potential values may result from measurement of volume-averaged pressures, which include both matrix and fracture water potentials; thus current measurements may not be able to resolve small-scale water potential variations. Uniform water potential values are not consistent with the presence of preferential fluid flow paths and film flow in fractures.

The water chemistry at Yucca Mountain is controlled by many physical and chemical processes, including the rate of infiltration, evapotranspiration, matrix-fracture interaction, mineral dissolution and precipitation, ion exchange and sorption, mixing, and liquid-gas interaction. While many components of fluid flow and reactive transport in a heterogeneous fracture-matrix system are currently incorporated in numerical simulations (e.g., Sonnenthal and Bodvarsson 1999; Xu et al. in press), improvements in conceptual and numerical models are needed to better capture the coupled effects of these processes.

Impact/Importance to the Yucca Mountain Project

Aspects of Yucca Mountain water chemistry data may significantly impact current performance assessment models. Pore water compositions at Yucca Mountain vary both spatially and temporally under natural conditions; this variability is reflected in the composition of secondary minerals that have precipitated from fluids within the UZ (Figure B-2). Even greater variability would result from the emplacement of high-level waste in a potential repository, and thus it is critical that coupled process models are utilized to predict the range of possible seepage compositions that could interact with waste packages.

Pore water compositions are in part a function of climate, with more dilute compositions resulting from higher precipitation and lower amounts of evapotranspiration occurring during colder, wetter glacial stages. Models using geochemical fluxes of chloride found in porewater samples result in calculated current infiltration rates that can be as low as 1–2 mm/yr (BSC 2002, South Ramp samples from Table 26). A time-averaged infiltration rate of approximately 6 mm/yr was calculated using the reported calcite abundance in cuttings from WT-24 and a reactive transport model of UZ flow (Xu et al. in press). These interpreted infiltration rates suggest that climate models used in total system performance assessment may yield conditions that result in overestimates of infiltration rates. Lower infiltration and fluid flow rates within the UZ would decrease the probability of seepage, and therefore lead to improved predicted performance of the potential geologic repository at Yucca Mountain.

The apparent chemical disequilibrium between the perched water bodies and porewaters in nearby unsaturated rocks at Yucca Mountain (e.g., Meijer 2000) suggests that the rate of water flow in the fractures differs from that in the matrix. The pore water chemical signature probably reflects an average of variable compositions of fracture waters that have passed through the matrix blocks over long periods of time (up to 10,000 to 100,000 years), and is also affected by water-rock matrix chemical interactions. Chemical disequilibrium may also occur between fracture water in fast-flow paths and adjacent matrix porewaters within the UZ at Yucca Mountain. Better characterization of matrix-matrix and matrix-fracture interaction will result in improved conceptual and numerical models to explain the observed variability of water chemistry and predict future flow and transport behavior at the potential repository.

Objective

Key factors affecting the performance of the geological repository at Yucca Mountain include the distribution of percolation fluxes and velocities over time and space, the location and importance of fast-flow paths, and the nature and extent of water-rock interaction and its effect on fluid flow and chemical transport within the UZ. Field measurements of rock fracture and matrix hydrogeologic properties, water saturations and matric potentials, and determination of variations in fluid chemistry throughout the different hydrogeologic units at Yucca Mountain are used to constrain numerical models that predict fluid flow and reactive transport behavior for the potential repository. Accurate assessment of the hydrogeologic properties and conditions at Yucca Mountain and their incorporation into coupled-process numerical models are critical in predicting the long-term performance of the potential Yucca Mountain repository.

The goals of the proposed study center around the integrated use of field, laboratory and modeling studies to address the processes and issues concerning chemical and isotopic variations in water chemistry and differences in water potential within the UZ at Yucca Mountain.

Workscope

1. Use of isotopic data in evaluation of percolation rates and fast-path flow

   Incorporate isotopes (such as tritium, ^{36}Cl, ^{14}C, ^{18}O, D, $^{87}Sr/^{86}Sr$, and U-series isotopes) into geochemical models to better constrain fluid flow paths, percolation rates, and improve estimates of flowing fracture frequency at Yucca Mountain. Isotopic fractionation between gas, mineral, and liquid phases (for stable isotopes) and decay (for radiogenic isotopes) will be integrated into the model. These model refinements will allow for better estimates of time-averaged percolation rates at Yucca Mountain, thus helping with the selection of appropriate future infiltration rates for repository performance simulations (e.g., Yang 2002). Following these changes, models will be constructed and run to evaluate fast-flow paths and estimate percolation rates at Yucca Mountain.

2. Heterogeneity in pore water chemistry

   Investigate changes in pore water chemistry along detailed traverses between perched water zones and surrounding unsaturated zones, and variations in pore water chemistry between nearby core samples for water extracted from welded tuff using an ultracentrifugation technique (this work conducted together with the USGS). These data would then be incorporated into stochastic transport analyses to address the origin of chemical heterogeneity. These studies would provide needed constraints for explaining persisting chemical variability in water chemistry over small distances, and help constrain estimates of water infiltration rates and flow paths in low permeability rocks.

3. Water-mineral interaction

   Use geochemical modeling to investigate how changes in water chemistry over time may result in episodic precipitation of secondary minerals in fractures and lithophysal cavities. Wilson and Cline (2001) observed an abrupt change from Mg-free calcite to sparry calcite with up to ~1.0 wt.% Mg in secondary calcite found in fractures and lithophysal cavities at Yucca Mountain. (The cause for this change in mineral chemistry has not yet been identified).

4. Water potential studies

   Evaluate water-potential data using inverse modeling techniques, and determine the feasibility of adapting existing bench-top laboratory techniques so that small-scale variations can be resolved in the field. Using numerical models, evaluate reliability of UZ psychrometer data and calculate solute effects on estimates of matric potentials.

Schedule

1. Use isotopic data in evaluation of percolation rates and fast-path flow

    1.1 Incorporate isotope systematics into geochemical models: Year 1

    1.2 Conduct simulations to evaluate percolation rates and fast-path flow: Years 2 and 3

2. Heterogeneity in pore water chemistry

    2.1 Obtain pore water chemistry from traverses between perched water zones and nearby UZ areas (in collaboration with USGS and LANC, if core is available: Years 1 and 2

    2.2 Create stochastic transport models: Years 2 and 3

3. Water-mineral interaction

    3.1 Geochemical modeling of episodic opal and calcite precipitation: Years 1 and 2

    3.2 Geochemical modeling of variability in secondary calcite composition: Years 1 and 2

4. Water potential studies

    4.1 Inverse modeling of existing water potential data: Year 1

    4.2 Development of new field methods to measure water potential: Years 2 and 3

    4.3 Use numerical models to evaluate psychrometer data and solute effects: Years 1 and 2

Product

The results of each of the workscope items will be published in internal reports and peer-reviewed journals. The key findings will be incorporated into all models that feed into TSPA.

Level of Effort

Task 1: 1 FTE for Year 1, 1.5 FTE for Years 2 and 3

Task 2: 1 FTE for Year 1, 1.5 FTE for Years 2 and 3

Task 3: 1 FTE for Years 1 and 2

Task 4: 1 FTE for Year 1, 0.5 FTE for Years 2 and 3

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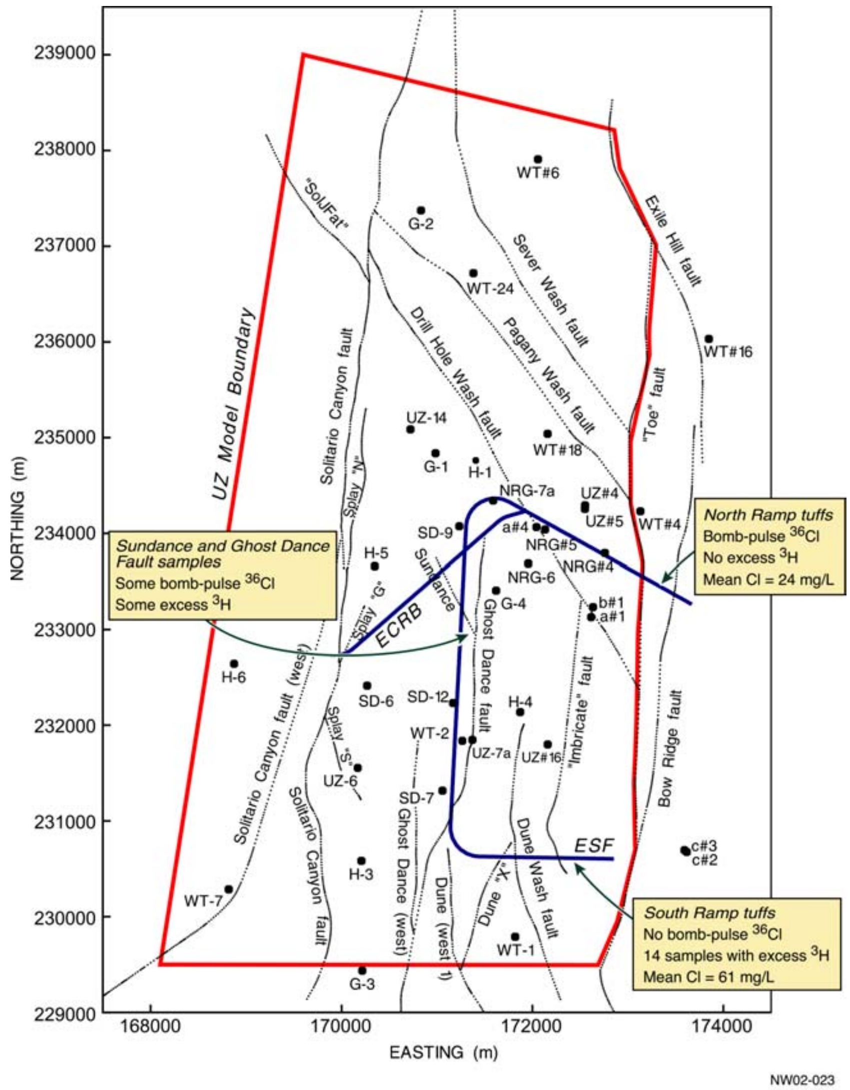


Figure B-1. Geochemical evidence for fast flow at Yucca Mountain. Data for South Ramp, North Ramp, and fault zones from BSC 2002 (Sections 6.6.3.3, 6.6.6.4, Tables 13, 14, 26), BSC 2001 (Appendix B, Section 3.5.3). Lack of detectable bomb-pulse ^{36}Cl in the South Ramp area may in part be due to higher Cl contents for porewaters in this area.

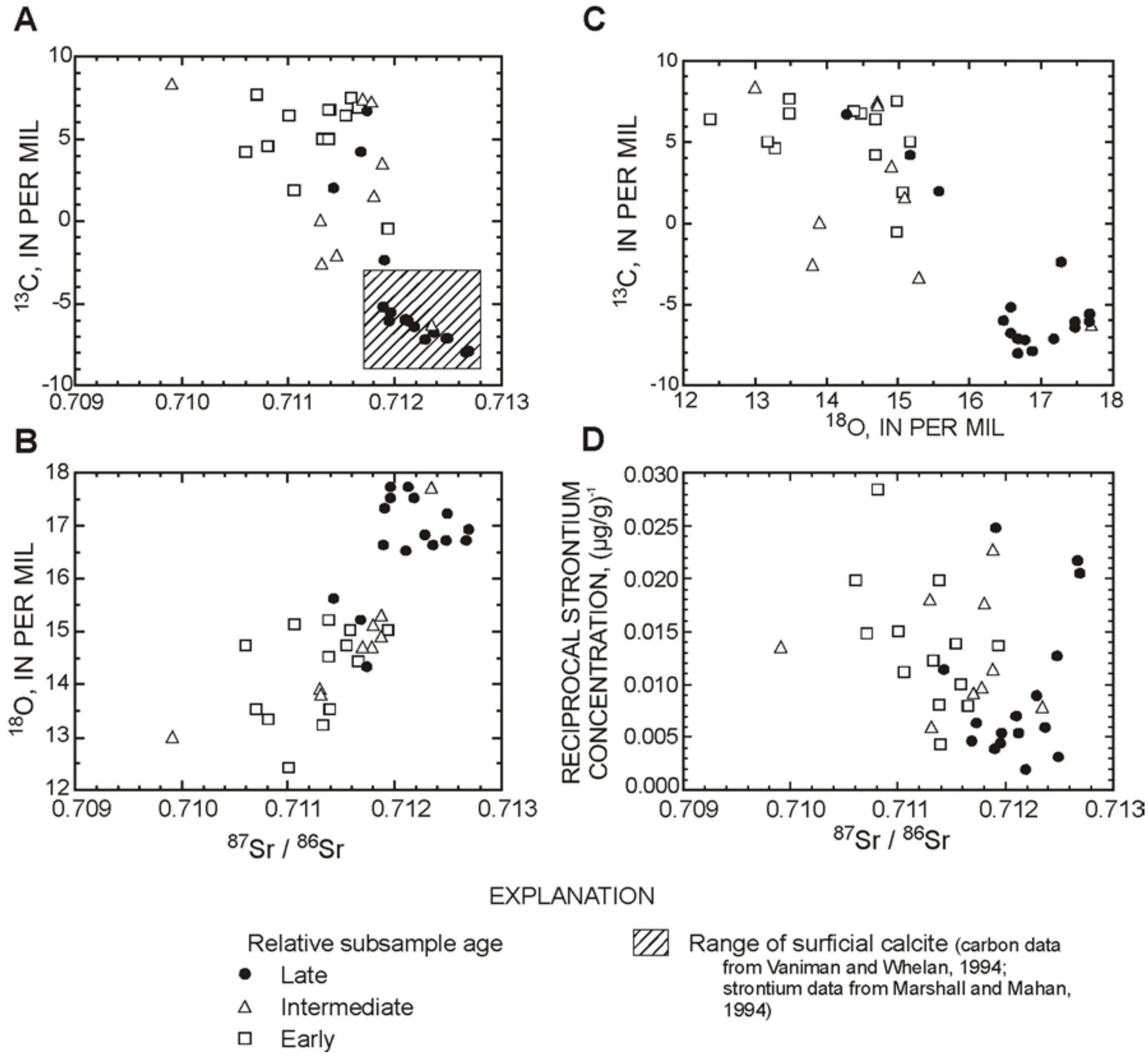


Figure B-2. Trends in secondary calcite compositions from the ESF with time (from BSC 2002, Figure 64)

1C.Water Flow Mechanisms in the Unsaturated Zone at Yucca Mountain: from Pore-scale Flow to Drift- and Large-scale Flow Processes

Focus Area: Unsaturated Zone
Contact: Jens T. Birkholzer, JTBirkholzer@lbl.gov, (510) 486-7134
Collaboration: LBNL

Statement of Problem

Unsaturated flow in fractured rock at Yucca Mountain has generally been treated with continuum concepts, using averaged input properties and simulating averaged physical processes. In such concepts, pore-scale and fracture-scale processes are not explicitly considered, which may lead to an underestimation of the probability that episodic, highly localized pathways develop. These pathways may carry liquid water at flow rates much larger than average percolation. Recent experimental and modeling studies have indicated that the occurrence of intermittent rapid flow events may greatly affect the prediction of unsaturated flow at Yucca Mountain.

Impact/Importance to the Yucca Mountain Project

The unsaturated zone (UZ) above and below the repository horizon is considered to form a natural barrier with potentially great significance for the performance of the site. In most Yucca Mountain Project (YMP) studies, the effectiveness of this barrier has been evaluated using predictive models based on continuum concepts, e.g., the Drift Seepage Model for evaluating seepage into drifts, or the UZ Transport Model for studying radionuclide transport. However, a number of theoretical, laboratory, and field studies have recently demonstrated that flow patterns in unsaturated fractures may differ strongly from the time- and space-averaged flow assumed in continuum concepts. From these studies it became apparent that infiltrating water often proceeds through localized preferential flow paths. Also, flow was often observed to form in an intermittent, episodic manner (even for constant flow boundary conditions), induced by gravitational instability or aperture variations within the fractures. Some possible implications of these conceptual differences are explained in Figure C-1. The first schematic (A) shows the current understanding of unsaturated flow in the UZ, with a large number of fractures "actively" contributing to quasi-steady-state flow. Following this concept, small amounts of water would reach the repository horizon at numerous locations. The second schematic (B) shows rapid episodic flow events that would occur less frequently in time and space. At the repository horizon, water would be collected at fewer locations, but at much higher flow rates upon occurrence. The performance vulnerability of the natural barrier is highly influenced by the different flow patterns shown in Figure C-1.

Unfortunately, field evidence of ambient water flow at Yucca Mountain was found only once, upon excavation of Niche 1, not permitting determination of which of the two above flow concepts is more realistic. To account for these uncertainties in flow conceptualization, the possibility of localized episodic flow was introduced in the 2001 Supplemental Science and Performance Analyses (SSPA) analysis of drift seepage, in a fairly preliminary manner (BSC 2001, Section 4.3-2). The SSPA analysis was based on a very simple conceptual framework of how such flow events may form in the UZ and what their flow characteristics may be. This proposed work aims at improving the preliminary conceptual model and reducing the model uncertainty, by means of an in-depth laboratory and theoretical study analyzing the flow characteristics and the probability of episodic preferential, unsaturated fracture flow at Yucca Mountain. While this work can be essential for improving all predictive tools used to study the UZ, it is expected to be of major importance for analyzing the small-scale processes involved in drift seepage. Having more concrete information about flow patterns and their frequency in the repository host rock can lead to drastic changes in repository performance and more improved total system performance assessment models.

Objective

The inability of classical continuum approaches to capture localized episodic flow effects—along with their potentially significant impact on the predicted system behavior at Yucca Mountain—calls for a comprehensive research program with the following main objectives:

1. Develop a basic conceptual understanding of episodic preferential flow processes in fractures at Yucca Mountain, based on small-scale laboratory experiments and related pore-scale modeling study.

2. Evaluate the impact of episodic preferential flow on drift seepage in a systematic manner, for isothermal and thermal conditions, and provide input for performance assessment.

3. Study the potential impact of episodic preferential flow on model concepts used for large-scale simulations. Develop improved predictive modeling capabilities.

Workscope

The proposed research plan includes laboratory and modeling work to be performed on several scales. The different research components may be categorized into three main tasks, related to the three main research objectives stated above. See Figure C-2 for a schematic description of research tasks and their relation.

1. Pore-scale analysis of episodic preferential flow processes

   Develop a new conceptual understanding of small-scale unsaturated flow to explain episodic, intermittent rivulet flow occurring in single rough-walled fractures. Study is based on small-scale laboratory experiments and related pore-scale modeling work.

   1.1 Single fracture-replica flow experiments

   - Perform systematic flow visualization laboratory experiments, using transparent fracture replicas from Yucca Mountain with heterogeneous aperture fields and video equipment. Determine mechanisms (gravitational instability, capillary variation) leading to episodic rivulet flow and identify key geometric and hydraulic parameters. Focus on low-infiltration conditions to resemble hydrologic situation at Yucca Mountain.
   - Complement video visualization of preferential flow with advanced tomographic techniques (CT scanning, electrical resistivity tomography, seismic or radar tomography), as a testbed for experiments where visualization is not possible (see Task 3).
   - Study relative impact of matrix imbibition, fracture wall flow and contact angle using fracture replicas with different wall properties, i.e., impermeable fracture walls (glass faces) versus permeable wall (natural rock face on one side, opposite the video imaging tool).

   1.2 Pore-scale modeling

   - Develop a predictive tool to simulate pore-scale behavior of unsaturated flow.
   - Apply pore-scale models using stochastically generated fracture aperture fields. Compare model results to or calibrate against data from laboratory experiments. Examine potential for episodic and/or preferential flow using small-scale aperture variation, saturation, and percolation flux representative of conditions at Yucca Mountain. Provide ranges of parameters characterizing potential flow events (magnitude and duration) for Task 2.

2. Impact of episodic preferential flow on seepage into drifts

   Examine impact of episodic rivulet flow on seepage at isothermal and superheated conditions. Provide input for performance assessment. (Episodic flow events are expected to be particularly important for near-drift conditions, where small-scale processes can not be averaged).

   2.1 Episodic seepage at isothermal conditions

   - Evaluate performance of the capillary barrier at the drift wall for a range of localized episodic flow events estimated in Task 1. Perform small-scale laboratory experiments of flow in a fracture located above an open cavity. Develop a fully coupled model of small-scale unsaturated flow (capillary barrier effect) with in-drift conditions. Study geometric, hydraulic, and hydrodynamic conditions affecting the effectiveness of the capillary barrier.
   - Note: This workscope is closely related to Proposal E (Title: Capillary Barrier Effects, Film Flow, and Seepage from Drift Walls).

2.2 Episodic seepage at above-boiling conditions

- Evaluate performance of vaporization barrier for localized episodic flow events during the heated period (seepage is reduced as a result of vigorous boiling of water).
- Perform systematic flow visualization experiments for superheated fracture replica. Use setup similar to the isothermal experiments in 1.1, with test equipment placed into an incubator and heated to above-boiling temperature. Determine maximum penetration distance of finger flow before water has boiled off, and identify key geometric and hydraulic parameters.
- Derive conceptual model of thermal episodic seepage. Perform systematic study of properties representative of conditions at Yucca Mountain, using new model for thermal episodic seepage. Use range of localized episodic flow events estimated in Task 1.

3. New or improved conceptualization of unsaturated flow at increased scales

Study the potential impact of episodic preferential flow on flow behavior at increased scales. Evaluate how to incorporate these effects in large-scale model concepts. Compare pore-scale models, a discrete fracture network model, and continuum approaches. If necessary, develop new or improved conceptual models of large-scale unsaturated flow.

3.1 Multiple-fracture flow experiments and related modeling on a meter scale

- Perform flow infiltration experiments using the meter-scale block of fractured Yucca Mountain tuff. Conduct tomographic experiments to image the water flow in the fractures. (These remote sensing methods can be scaled up to field dimensions to verify the nature of fracture flow in drift-scale experiments). Evaluate potential of episodic preferential flow events at meter scale.
- Apply pore-scale models to meter-scale block. Examine unsaturated flow across fracture intersections. Compare model results to or calibrate against data from meter-scale block experiments.
- Develop new conceptual model for episodic preferential flow and front movement at larger scales that cannot be modeled with pore-scale approaches. Abstract results, determine effective parameters (if possible), providing input for 2D or 3D fracture network models. Perform detailed fracture network study for meter-scale block and compare results to data.

3.2 Large-scale fracture network modeling

- Examine fracture network information representative of Yucca Mountain.
- Apply fracture-network models on a larger scale (drift-scale to mountain-scale), using new or improved conceptualization of episodic preferential flow. Analyze results to obtain spatial and temporal flow focusing factors, relating local flow behavior to average percolation flux.
- Perform predictive studies of unsaturated flow using discrete fracture-network model/episodic rivulet model/continuum approaches. Compare results and validate model components, evaluate impact on large-scale modeling and performance assessment.
- Review all available field data as corroborating evidence to support model approaches. Identify characterization needs and develop recommendations for unsaturated fracture flow investigations. Propose validation strategies.

Schedule

1. Pore-scale analysis of episodic preferential flow processes

1.1 Single fracture-replica flow experiments: Year 1 and Year 2

1.2 Pore-scale modeling: Year 1 and Year 2

2. Impact of episodic preferential flow on seepage into drifts

    2.1 Episodic seepage at isothermal conditions: Year 3 and Year 4

    2.2 Episodic seepage at above-boiling conditions: Year 3 and Year 4

3. New or improved conceptualization of unsaturated flow at increased scales

    3.1 Multiple-fracture flow experiments and related modeling on a meter scale: Year 3 and Year 4

    3.2 Large-scale fracture network modeling: Year 3 and Year 4

Product

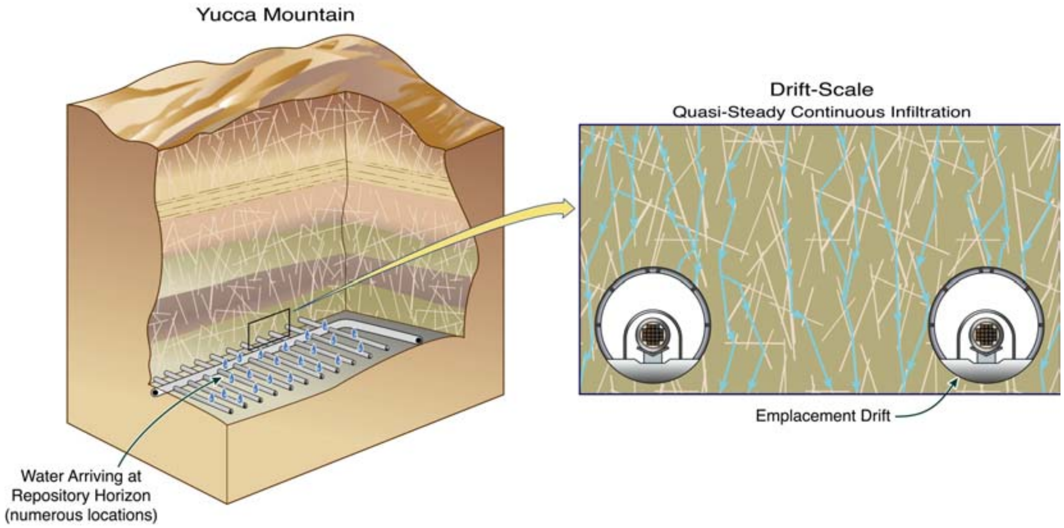
The results of each of the workscope items will be published in peer-reviewed journals. Progress reports will be produced on an annual basis, describing the scientific findings as well as proposed methods for implementation in TOTAL SYSTEM PERFORMANCE ASSESSMENT.

Level of Effort

The estimated resource for this work is 3.5 FTE for each Year 1 and Year 2, 3 FTE for Year 3, and 2 FTE for Year 4, plus material needed for setting up and conducting the experiments.

References

BSC 2001. FY01 *Supplemental Science and Performance Analyses*, Volume 1: Scientific Bases and Analyses. TDR-MGR-MD-000007 Rev 00 ICN 01.



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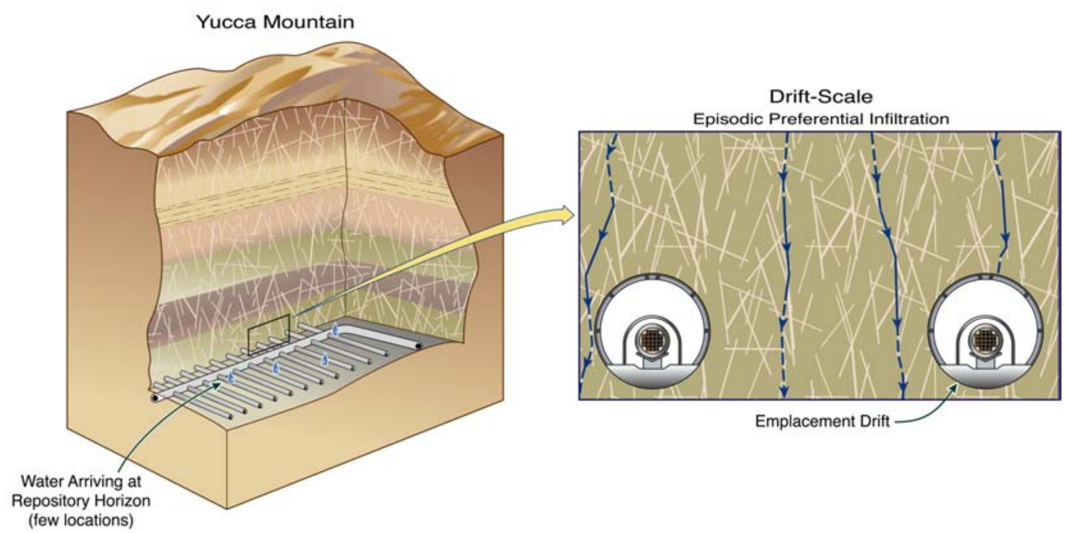

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Figure C-1. Schematic showing the different understanding of flow patterns in the UZ at Yucca Mountain
A: Infiltration patterns as modeled with continuum concepts
B: Infiltration patterns considering episodic preferential infiltration

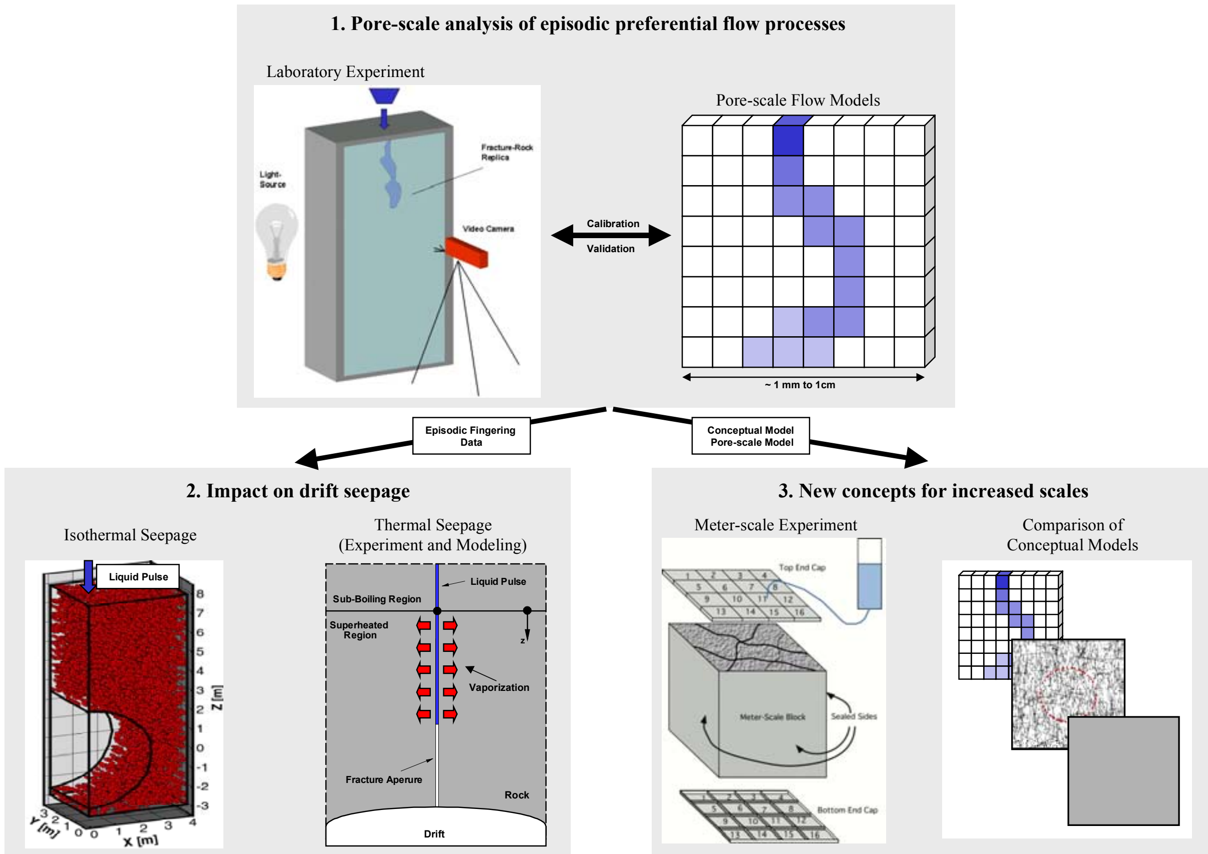

Figure C-2. Schematic showing the different research components and their relation

D. Feature and Fault Testing and Analysis

Focus Area: Unsaturated Zone
Contact: Joe Wang, JSWang@lbl.gov, (510) 486-6753
Collaboration: LBNL, potential collaboration with USGS and other BSC organizations

Statement of Problem

Based on the current understanding of Yucca Mountain, considerable redistribution of downward flow and transport occurs throughout the unsaturated zone (UZ), with substantial percolation diverted to faults before reaching the water table. Figure D-1a illustrates the concentration of flux along fault traces at the water table simulated by the current UZ Model. The fault contribution to flow and transport is based on permeabilities determined by air-injection tests at two fault locations away from the repository block (the Bow Ridge fault and the Ghost Dance fault, as illustrated in Figure D-2). The tests proposed focus on using liquid for all available faults, tuff interfaces, and other geological features along the ESF ramps, Main Drift, and ECRB Cross Drift. The liquid-determined permeabilities and tracer migration data will be used in the UZ Model to determine if the fault flow contribution is overestimated; distributions of geochemical data below the UZ boundary in the saturated zone (SZ) suggest that such an overestimation is possible. Figure D-1b shows that the chloride distribution in the SZ is smooth and does not have characteristics indicating that faults control the chemical distribution.

Impact/Importance to the Yucca Mountain Project

The performance of the UZ as a natural barrier depends on addressing the following important questions: (1) Above the repository, does significant diversion indeed occur globally (throughout the area) driven by lateral flows along interfaces to the bounding faults? Or does diversion occur locally around drift walls driven by a capillary-barrier mechanism? (2) Below the repository, does diversion to the faults focus the fast breakthroughs to a few localized release points at the water table? Or does dispersive transport through tuff units delay the breakthrough and/or smooth out and reduce radionuclide concentrations? The proposed program will address these uncertainties and significantly improve realistic representation of the flow and transport processes in the UZ barriers. Realistic representation provides more definite and scientifically defensible inputs to the total system performance assessment (TSPA) model.

Objective

The objective of the proposed program is to directly quantify flow permeabilities and tracer transport paths with liquid tracer injections for features and faults observed along the drifts. The liquid testing phase is proceeded by an air-injection and geophysical imaging phase and followed by a post-thermal-stress testing phase. The feature and fault testing program will also emphasize integration with associated modeling to evaluate the capacities of faults as potential fast paths and features as effective diverters. The results will substantially remove the uncertainties in our current understanding, based on air-injection data from faults.

Workscope

The proposed field-testing program will focus on features and faults along the drifts, conducting tests in test beds along the drift walls using borehole clusters. The boreholes will be long enough to test the features away from the influence of the drift. Near the borehole collars, tests will also be conducted to evaluate the flow paths for diverted flow around the drifts. The pneumatic and hydrological testing approach will be complemented by high-resolution geophysical imaging and by local borehole (postflow characterization) thermal stressing. After the active testing phase, borehole clusters will be used for monitoring to develop the equipment and approaches needed during the performance confirmation period. The testing and monitoring program will include an associated modeling component to further enhance the integrated, multidisciplinary approach needed for the repository program.

Geological information mapped along the ramps, drifts, alcoves, and niches will be evaluated to determine test locations, the extent of the test bed, borehole cluster configuration, and all other relevant information for inputs to the pre-test design. Figure D-2 illustrates the likely locations for the Sundance fault (three locations: in the ECRB Cross Drift, the ESF Main Drift, or Alcove 6), the Drillhole Wash fault (the North Ramp), the Ghost Dance fault (three locations: Alcove 6, Alcove 7, or the southern part of ESF), the Solitario Canyon fault (one location), an unnamed fault with 5 m offset (at ECRB 22+38), and the South Ramp faults (multiple locations). These locations will all be investigated, along with tuff interfaces and other features.

1. Test Bed Characterization

   Crosshole pneumatic testing in boreholes will directly map out the potential flow-path connections, using boreholes instrumented with packers. Permutations of injections and detections of pressure pulses with gas tracers will be used to measure the air-permeability distribution and effective porosity values. High-resolution crosshole geophysical-imaging techniques can also be used in the drilled boreholes to characterize the test beds, confirm the mapped features, and detect hidden cavities or structures in the planned test areas.

2. Borehole Design and Liquid Testing

   For nearly vertical faults, one set of boreholes will likely be drilled within the fault plane, with another set drilled perpendicular to the fault plane. Two or three in-plane boreholes are planned to be horizontal, with spacing of 2–3 m, and other boreholes may be slanted 30–45^{o} to reach larger spatial separation between borehole intervals, as illustrated in Figure D-3a. The in-plane liquid testing directly characterizes the spatial channeling of fluid flow and tracer transport flow paths (Dahan et al. 1999). For tilted interfaces, boreholes in the plane will be drilled normal to the dip. Additional off-plane boreholes will be drilled above and below the features, as illustrated in Figure D-3b. For these two types of borehole-cluster-based test beds, the drilling can be launched directly from existing drift or alcove space, or from a simple drill bay routinely excavated for other utility functions along heavy traffic drifts. For some specific feature evaluations, such as the Crest Alcove needed to replace the ECRB bulkhead study to observe seepage below the Yucca Mountain crest in areas without PTn coverage, dedicated excavation will be required. This proposed program will support the evaluation and design for this and other special-purpose evaluations.

   Upper borehole intervals will be used for liquid releases, while lower borehole intervals will be used for flow quantification and tracer sampling. Tests with saturated borehole intervals will be followed by partially saturated tests at lower injection rates. The difference between injected and collected masses will be used to assess how effectively flow is confined within the fault or feature, to quantify imbibition into surrounding rock, and to estimate flows that are diverted or that escape from the test bed. Supplemental drilling may be needed to confirm and map the plume configurations. If slot-cutting techniques are found to be feasible and cost-effective after a few years of development at ESF, slots will be added to the program for better mass-balance testing.

3. Thermal Testing

   After the hydrological testing phases, localized heat sources will be placed at selected borehole intervals to evaluate the permeability changes induced by thermal-mechanical and coupled processes. Air-permeability tests will be conducted before and after heating phases to quantify the changes.

4. Borehole Monitoring

   After the boreholes return to near-ambient conditions, packers or other borehole sensors will be placed in the boreholes for long-term monitoring. The objective is to develop long-term monitoring techniques for *in situ* condition changes around waste emplacement drifts. The sensors need to have the capacities to sustain high temperature, maintain wireless communication for data download, and perform *in situ* calibration, among other requirements.

5. Laboratory Support

   Concurrent with the field-testing activities, laboratory testing will measure core properties and chemical/isotopic changes of fluids collected during testing. The laboratory-testing program contributes to process understanding of different effects observed in the field. A newly developed portable x-ray apparatus may be deployed in the field for core characterization (matrix porosity, lithophysal cavity porosity, rock texture, fracture density).

6. Modeling and Assessment

   Modeling plays an essential role in the testing program. Models will be used to design the tests, interpret the results, quantify the processes, and analyze the correlations among different features. The modeling studies will also include assessment of responses to extreme conditions, through the use of various scaling and extrapolation techniques. The extreme conditions include the episodic concentration of extreme inflow from the ground surface in future wet climates along washes.

Schedule

The total duration of feature and fault testing and the complementary analysis program is five years. The active testing phases for each location is three years, with Year 1 spent on test bed construction, geophysical characterization, air-permeability testing, and pre-test prediction; Year 2 on liquid flow and transport testing; and Year 3 on thermal testing. In Years 4 and 5, the first test bed boreholes will be instrumented for monitoring. The test bed startup will spread over the first three years, with Year 1 effort focusing on Sundance fault and available Ghost Dance fault locations; Year 2 effort focusing on the South Ramp faults, the high fracture zone, and the cavity-rich zone; and Year 3 effort focusing on the Solitario Canyon fault, the unnamed 5 m offset fault, and the Crest Alcove, all behind the ECRB bulkheads.

	Test Bed Characterization	Liquid Testing	Thermal Testing	Borehole Monitoring	Laboratory Support	Modeling and Assessment
Year 1	N ESF*				N ESF	N ESF
Year 2	S ESF**	N ESF			N&S ESF	N&S ESF
Year 3	W ECRB***	S ESF	N ESF		All sites	All sites
Year 4		W ECRB	S ESF	N ESF	W ECRB	All sites
Year 5			W ECRB	N&S ESF		All sites

* N ESF for sites in the northern part of repository block, e.g., Sundance fault in ECRB, ESF, or Alcove 6; Drillhole Wash fault in the North Ramp, Ghost Dance fault in Alcove 6; PTn-TSw interface, Upper-Middle TSw interface, Middle-Lower TSw interface.

** S ESF for sites in the southern part of repository block, e.g., Ghost Dance fault in Alcove 7 and ESF; South Ramp faults, extensively fractured zone.

*** W ECRB for sites behind ECRB bulkheads, e.g., 5 m offset fault, Solitario Canyon fault, Crest Alcove, Lower lithophysal-nonlithophysal TSw interface.

Products

Products will include peer-reviewed journal articles for fault, feature, and fracture evaluations and comparisons. Annual reports will be submitted to document the progress and provide inputs to the revision of the AMR on *In Situ* Testing of Processes (BSC 2001), as well as periodic data packages for inputs to UZ models.

Level of Effort

Five FTEs annually for 5 years: 2 FTE for test bed characterization (with air-injection, geophysical imaging) and borehole monitoring, 2 FTE for hydrological testing, thermal testing, and lab support, 1 FTE for modeling, analysis, and assessment.

References

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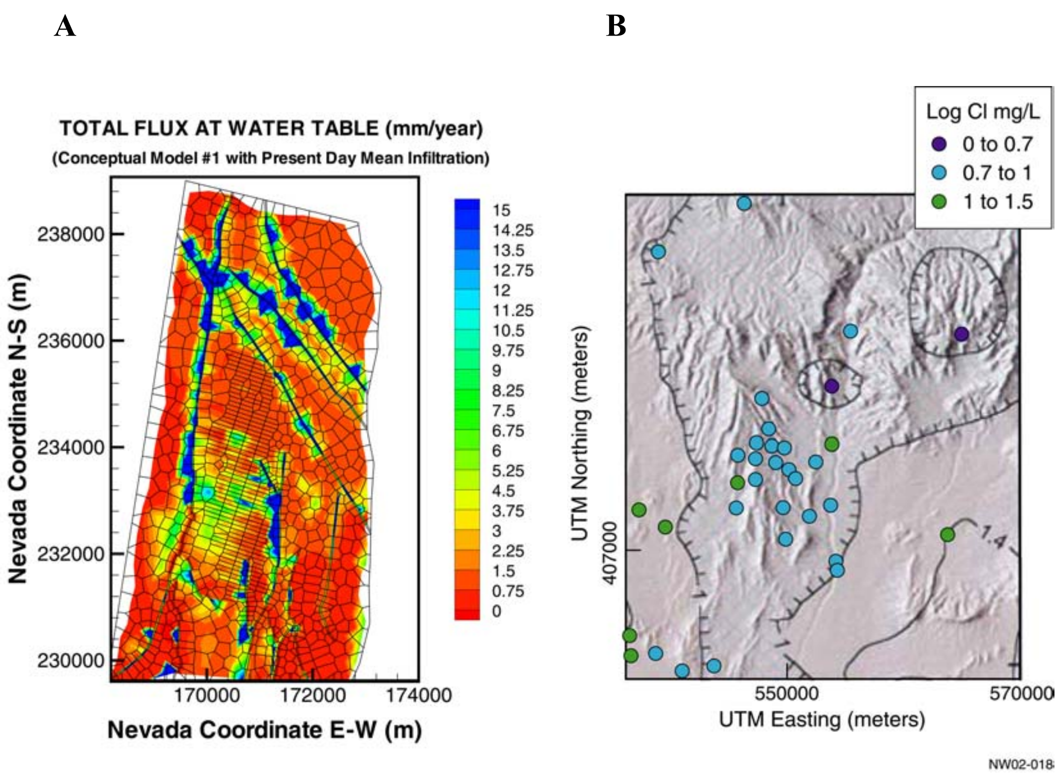


Figure D-1. Comparison of the distribution difference between (A) percolation flux reaching the water table, and (B) chloride concentration in the saturated zone at Yucca Mountain.

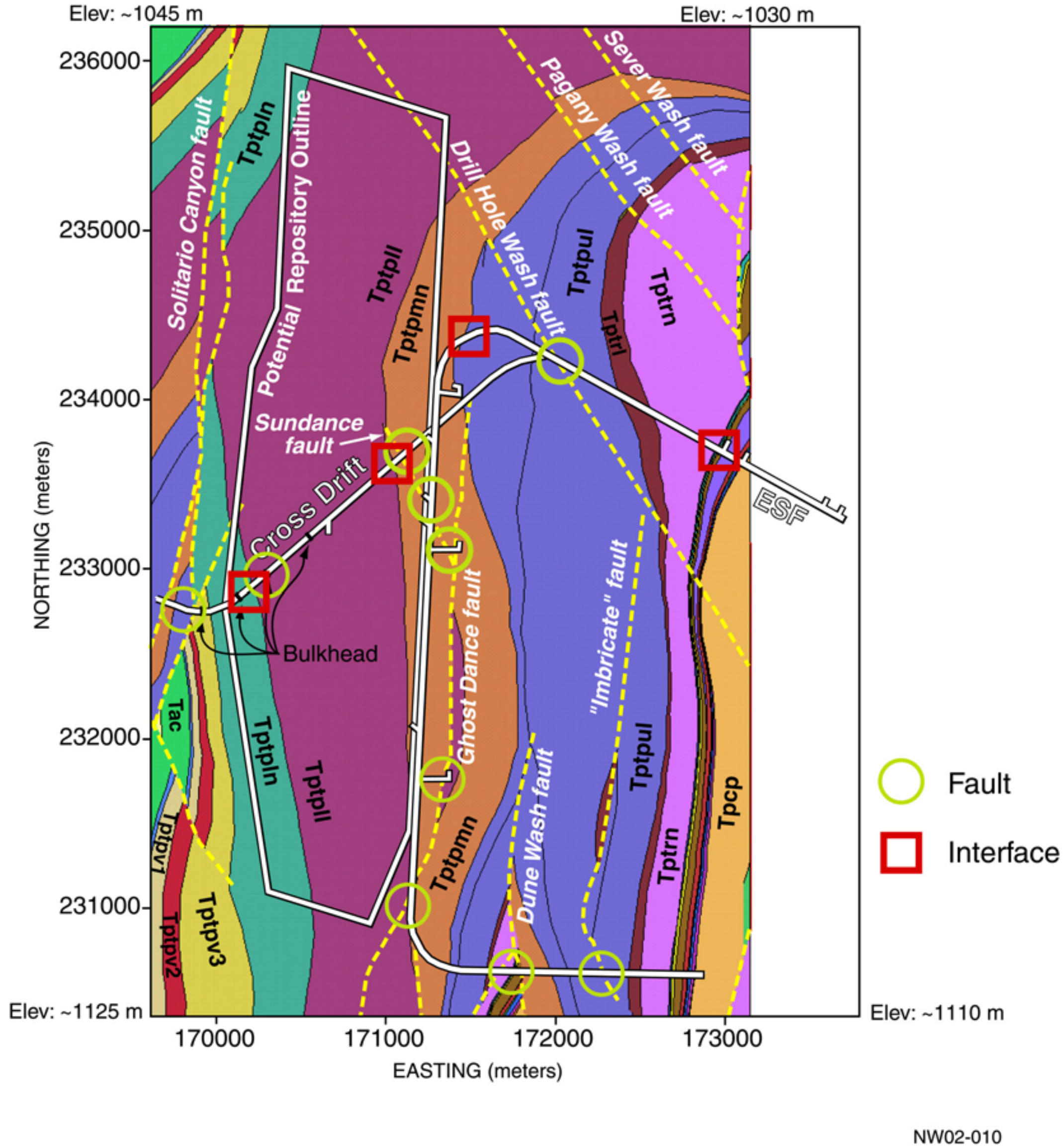
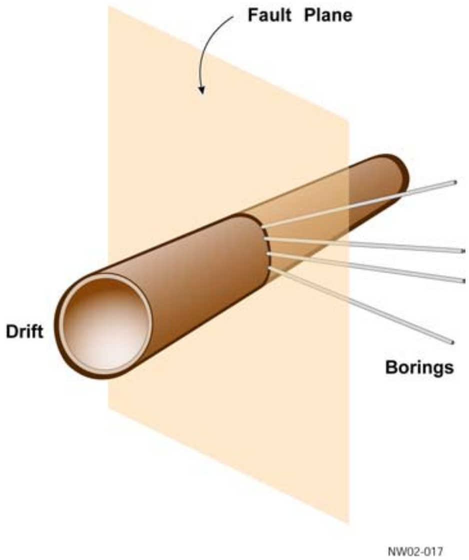


Figure D-2. Feature and Fault Locations in the ESF Ramps, Main Drift, and in the ECRB Cross Drifts.



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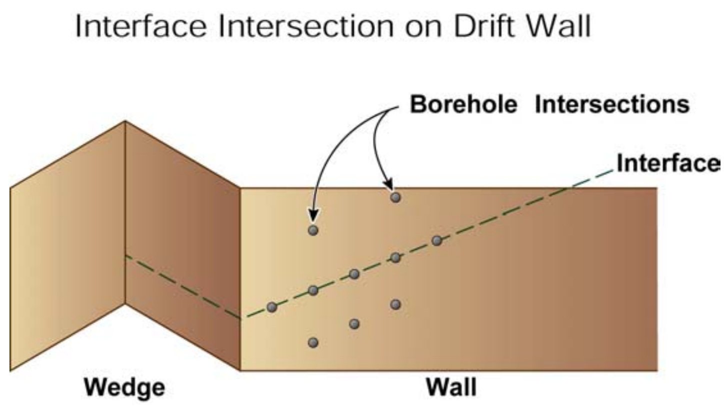

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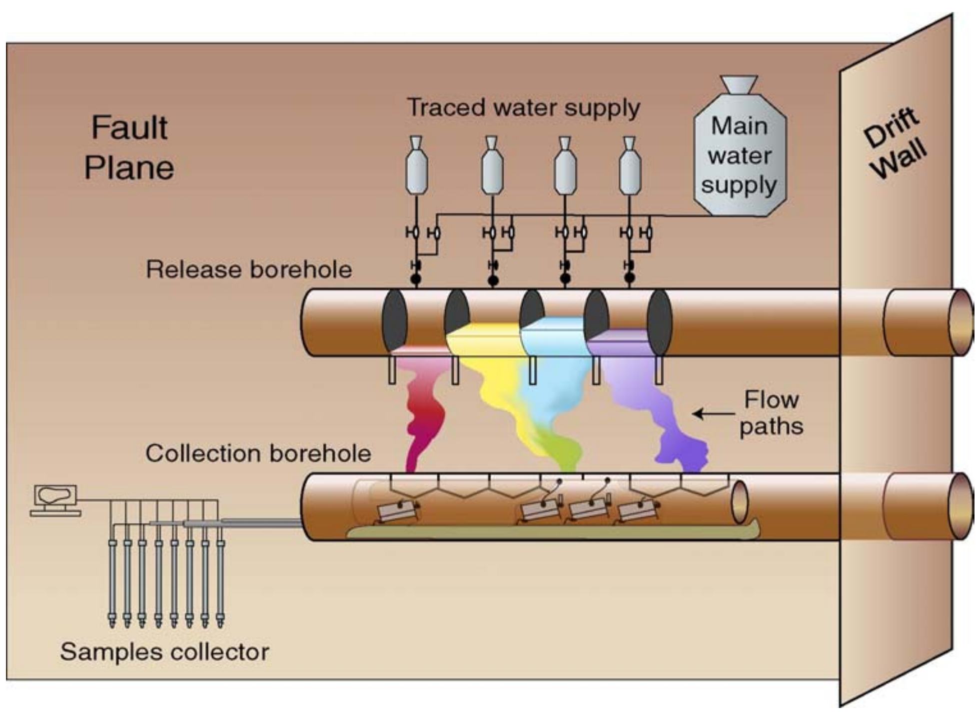

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Figure D-3. Schematic Illustration of (A) Fault Testing, (B) Tuff Interface Testing, (C) Conceptual Liquid Release and Tracer Collection Cross-Hole Testing Layout.

E. Capillary Barrier Effects, Film Flow, and Seepage (Dripping) from Drift Walls

Focus Area: Unsaturated Zone
Contact: Tetsu Tokunaga, TKTokunaga@lbl.gov, (510) 486-7176
Collaboration: LBNL

Statement of Problem

Whether and to what extent seepage into drifts will occur, under various scenarios of percolation fluxes, are issues critical to the viability of Yucca Mountain as a nuclear waste repository. Seepage becomes a critical issue if and when the matric (capillary) potential is near-zero along portions of drift walls and ceilings. Under such conditions, capillary barrier effectiveness becomes limited, and interrelations between local percolation and evaporation rates, wall (and ceiling) topography, and film flow will determine the extent (if any) of seepage. Of these factors, the interactions between wall topography and inclination, film flow, and seepage are the most complex. Yet whether percolating water bypasses canisters via film flow along drift walls or drips onto canisters (seepage) is critical to successful waste isolation (Figure E-1). Thus, these two modes of liquid water flow in drifts need to be quantitatively understood. A related aspect of this problem involves influences of drift wall degradation and the presence of lithophysal cavities (Figure E-2). These latter phenomena alter the near-drift flow field and amplify larger scale wall roughness, thereby altering seepage fluxes.

Impact/Importance to the Yucca Mountain Project

The proposed research will quantify the extent to which film flow will diminish seepage into Yucca Mountain drifts, and estimate the extent to which wall degradation will alter the partitioning between film flow and seepage. This information is needed to improve estimates of effective seepage (dripping) into drifts since gross estimates based on subtracting evaporative losses from local percolation rates overlook the potentially major effect of film flow bypass. Thus the proposed research will substantially decrease estimates of effective seepage onto waste packages, and reduce associated uncertainties by properly removing the contribution of film flow.

Objective

A basic issue to be resolved is the partitioning of net water flux leaving drift walls (local percolation flux minus evaporation flux) between actual seepage (dripping) and film flow. Here, film flow is defined as a macroscopic process, encompassing effects of capillary channels and adsorbed water films (Tokunaga and Wan, 1997). This scientific problem encompasses aspects of thick film hydrodynamics, interfacial physical chemistry, and unsaturated-saturated flow. Objectives specifically related to modeling flow and seepage responses to drift degradation and lithophysal cavities include (1) understanding the effects of fracture dilation on seepage rate and flow paths around drifts, (2) understanding the effects of the rockfall and extended rock failure on the seepage and flow around drifts, and (3) understanding the influence of lithophysal cavities on seepage and flow fields.

Workscope

Major issues to be resolved are the capacity for film flow along drift ceilings and walls, and criteria associated with dripping. This work has various facets, but can be broken down into (1) tasks directly addressing mechanistic aspects of film flow and seepage, and (2) tasks associated with numerical modeling of flow field changes due to fracture dilation, rockfall, and lithophysal cavities.

1. Mechanics of film flow and seepage

   In order to obtain results that have direct relevance to Yucca Mountain, the main studies will be done on tuff samples from the Yucca Mountain repository horizon. To connect these studies to a broader context, they will also be linked to ongoing studies of film flow scaling being conducted on model (statistically geometrically similar) surfaces. The actual drift surface represented by individual experiments and model calculations will be specified by their surface orientation (inclination) as shown in Figure E-1. Details of most experimental methods have been published (see reference list). Simulated UZ pore waters will be used in all experiments.

1.1. Local film flow capacity (macroscopically flat surfaces)

These studies will be done on macroscopically flat tuff surfaces, with root mean-square roughnesses (RMSR) in the range of 0.1 to 1 mm. A slight variation in the flow cell described in Tokunaga and Wan (1997) is used to establish isobaric (uniform matric/pressure potential) flows at various prescribed inclinations. The threshold flux density associated with dripping is determined as a function of inclination angle.

1.2. Regional film flow capacity (larger roughness, longer wavelength surfaces)

These studies will be done on larger (100's of cm^2 surfaces), that include larger amplitude roughness features. Their RMSR will be in the range of 10 mm. Some of the test samples will be obtained from the cubic meter block. The same type of flow cell described previously will be used to establish macroscopically isobaric flows at various prescribed inclinations. The threshold flux density associated with dripping is determined as a function of inclination angle and larger-scale roughness. Additional tests at this scale will be done directly on the cubic meter block.

1.3. Integration

Correlations between macroscopic surface orientation, surface roughness and dripping threshold will be obtained experimentally. These integrated results will be included in drift seepage models (Task 2). Results will also be compared with predictions of dripping thresholds based on a topography-potential model (Tokunaga et al., in preparation), as well as other improved models to be developed during the course of the proposed research.

2. Modeling of flow field changes due to fracture dilation, rock fall, and cavities

2.1. Effects of fracture dilation

Because of excavation, stress is relieved at the drift, and fractures are expected to dilate at certain areas around the drift. Such fracture dilation depends on the orientation of the fracture set and generally occurs within one drift radius. An increase in fracture aperture generally causes an increase in fracture permeability and a decrease in $1/\alpha$ value. The measured increase in permeability from the pre-excavation to the post-excavation values is a result of this effect. A three-dimensional numerical model will be applied to estimate the seepage enhancement.

2.2. Effects of rockfall and extended rock failure

Rockfall probabilities in the drifts under various scenarios will be generated, based on fracture maps in the ESF at Yucca Mountain. To study the effect of rockfall on seepage, two calculations will be considered, one in which a rockfall block was taken out from the crown of the drift, and the second in which a rockfall block was taken out at the spring line (Figure E-2, two upper cases). Over time, extended rock failure may occur at the ceiling of the drift. A long-term performance prediction of the extended rock-failure probability is needed. This is schematically represented by the lower-right part of Figure E-2. Using 3-D degradation profile scenarios, simulations will be made to evaluate the impact of extended rock failure on seepage. Partitioning between actual seepage and film flow will be estimated based upon analyses of laboratory experiments (Tasks 1.2 and 1.3).

2.3. Effects of lithophysal cavities

In general, seepage into drift depends on details of the heterogeneity in the vicinity of the drift, which acts as a capillary barrier. Local heterogeneities such as lithophysal cavities can permit seepage through locally focussing flow. Proper conceptual models are needed to describe the lithophysal cavities. Then the cavities will be distributed into a 3-D stochastic permeability field.

More simulations are used to calculate a set of results using multi-realizations. The spread from the multi-realizations should provide an indication of geostatistical variation.

Schedule

Year 1	Year 2	Year 3
Task 1.1 Task 2.1	Task 1.2 Task 2.2	Task 1.3 Tasks 2.2 and 2.3

Products

Journal articles will be published, and an annual progress report will be provided to DOE.

Level of Effort

3.5 FTE per year.

Materials and equipment: Yucca Mountain tuff samples, syringe pumps (2), peristaltic pumps (2), pressure transducers (20), and data logger (1).

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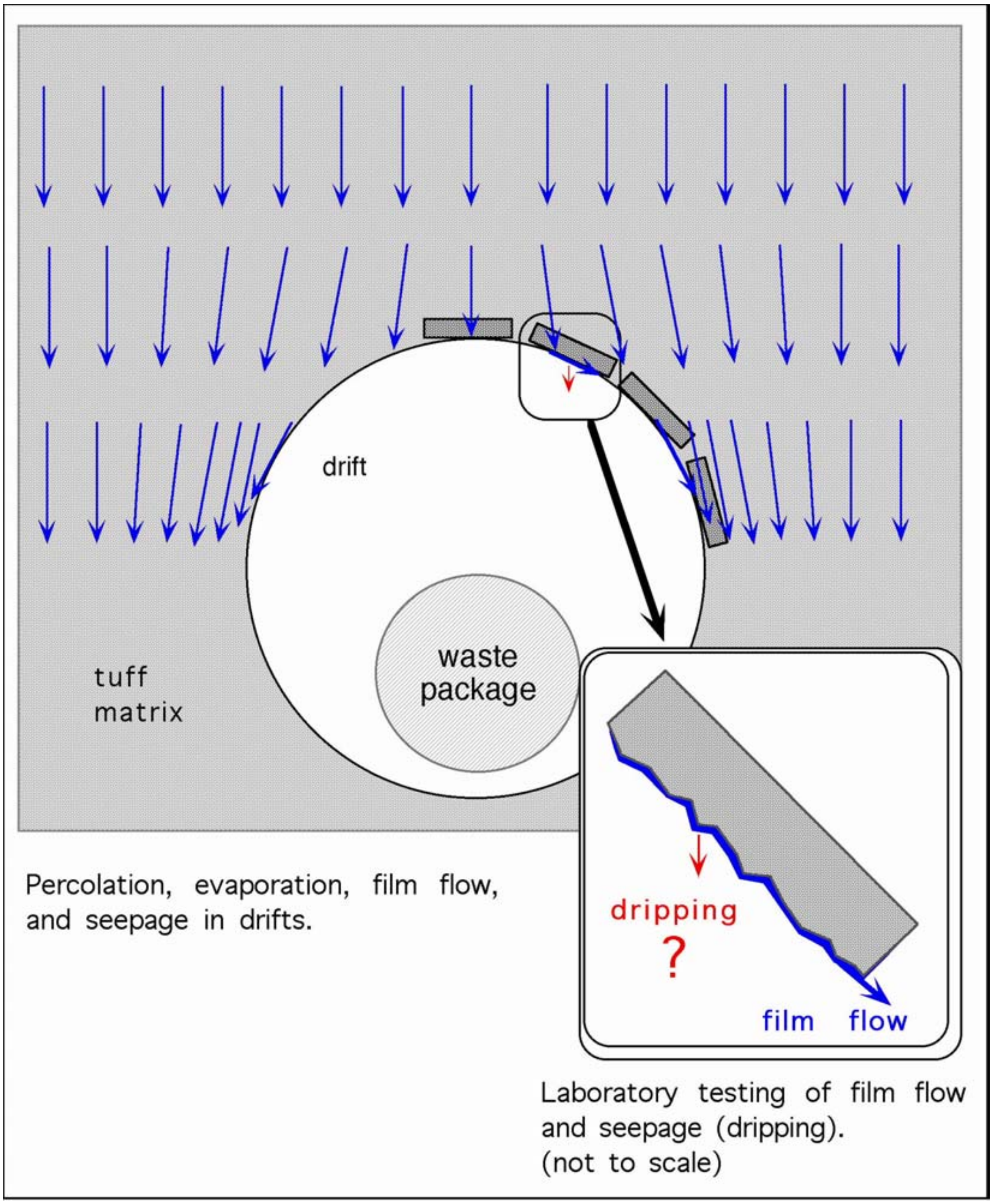

Figure E-1. Flow in the drift environment, and laboratory testing of partitioning between film flow and effective seepage (dripping).

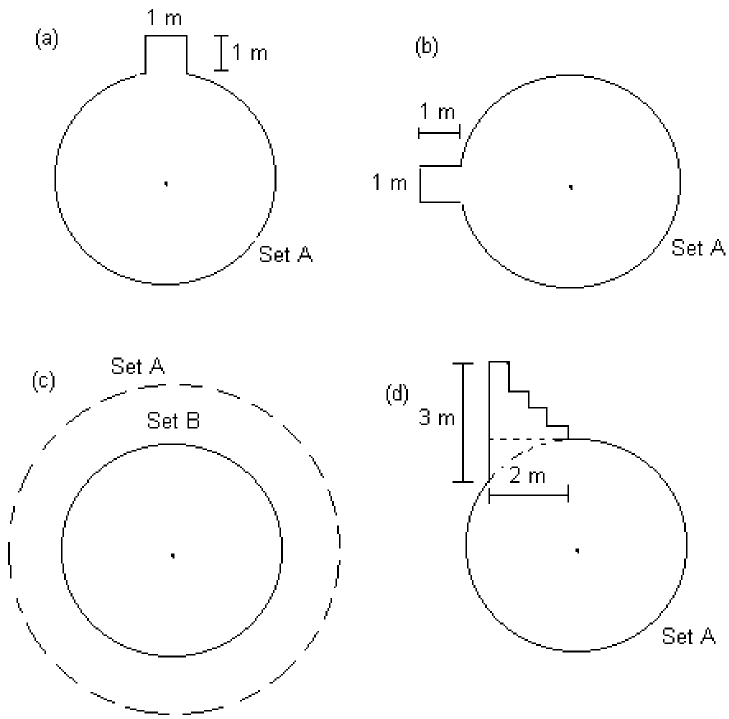

Figure E-2. Drift-degradation submodel scenarios: fracture dilation (c), rockfall from the drift ceiling (a) and from the springline (b), and extended rock failure (d) (from Li and Tsang, 2002).

F. Experimental and Modeling Study of Near-Drift Moisture Dynamics

Focus Area: Near Drift
Contact: Rohit Salve, R_Salve@lbl.gov, (510) 486-6416
Collaboration: LBNL with Testing Coordination Office

Statement of Problem

Knowledge of flow and transport processes affecting near-drift moisture dynamics at Yucca Mountain is critical for assessing the performance of natural and engineered barriers. Such knowledge is key to preventing corrosion of waste packages and mobilization of radionuclides. The rate and amount of water migrating into a drift is largely controlled by both natural flow phenomena and anthropogenic alterations, such as geometry of the excavated drift and intradrift microclimatic perturbations. At the same time, in-drift conditions, such as ventilation and heating, are likely to affect the flow and transport through fractured tuff in the near-drift zone. A schematic of flow and transport processes in fractured tuff in the near-drift zone is shown in Figure F-1. These processes are expected to affect the in-drift microclimate and are themselves affected by in-drift microclimate conditions. Since the excavation of the Yucca Mountain Main Drift in 1996, no naturally occurring seeps have been observed in the Exploratory Studies Facility (ESF). Rather, a 1-2 meter "dryout zone" has been observed to spread radially from the tunnel. Despite no observation of continuous natural seeps in the cavities and tunnels excavated at Yucca Mountain, dripping water has been observed to occur sporadically at rock bolts located in holes drilled with water. Seepage has also been observed along the ceiling of excavated cavities during infiltration experiments involving water introduced into the fractured rock above these cavities (e.g., Salve et al, 2002; Salve and Oldenburg, 2001).

Ongoing moisture monitoring studies along the terminal 944 m of the Cross Drift at Yucca Mountain, carried out since 1999, have indirectly shown the existence of liquid water (based on the presence of rust spots and organic growths) after the drift was isolated from ventilation (Figure F-2). During this study, films and beads of water have been observed along sections of the drift wall, as well as rapid increases in humidity and mold populations. Although observations clearly indicate the likelihood of liquid water accumulating in emplacement drifts, the dynamics of flow processes in and around the drift zone, and water accumulation and seepage into the drift, remain essentially unknown.

Impact/Importance to the Yucca Mountain Project

Existing modeling studies have shown that redistribution of moisture in the near-vicinity of and inside emplacement drifts is likely to result in liquid water appearing on waste packages, potentially accelerating degradation of the waste cladding. This study, which will investigate flow and transport processes affecting moisture dynamics in the proximity of waste emplacement drifts, is essential for evaluating the amount of moisture that can potentially affect waste package corrosion. Results from this type of investigation are needed for both determining the effectiveness of the near-drift environment as a natural barrier and for designing engineered barriers. For example, information about the spatial and temporal distribution of moisture through the rock surrounding the drift and into the drifts will help in designing protective shields surrounding waste packages. By investigating the nature of formation dryout associated with in-drift ventilation and creating in-drift microclimates resulting from the configuration of drifts, this study will provide design options for ventilated or nonventilated drifts.

Objective

The overall objective of this project is to identify mechanisms leading to the migration of water (liquid and vapor) in the vicinity of emplacement drifts. Specifically, the goals are to:

1. Identify conditions resulting in the transformation between liquid- and vapor-phase moisture (evaporation and condensation processes) in the near-drift environment.

2. Confirm whether seeps within the repository horizon exist, and monitor the spatial and temporal distribution of seepage and its chemical composition.

3. Assess the chemical and microbiological compositions in gases and water present in the emplacement drifts and determine how chemical and microbiological activity may affect moisture dynamics in the near-drift environment.

Workscope

This project will include two components: (1) field monitoring and experiments, and (2) numerical modeling investigations.

1. Field Experiments

   Monitoring of near-drift flow processes (e.g., evaporation, condensation and seepage) will be conducted along sections of the drift that include various rock formations and faults. Monitoring of naturally occurring seeps will also be conducted using 30–40 m long boreholes located in sections of the repository horizon deemed to be areas of relative high seepage (e.g., the high infiltration zone located near Station 20+00 in the Cross Drift). The drift and boreholes will be monitored with a newly developed remote-control "sensor buggy," loaded with sensors to measure water potential, saturation, relative humidity and temperature, and with a special video camera for monitoring seepage. This assembly will periodically traverse the length of drifts and boreholes to specified damp or dripping sections. Possible seep zones identified by the sensors will then be isolated and instrumented for long-term monitoring of liquid and gas hydraulic and chemical characterization. If needed, geophysical (ground penetrating radar, neutron, and seismic) logging/tomography will be used to monitor locations where water or elevated air moisture might be present.

   Microbial populations will be studied in the near-drift environment to develop an understanding of how biogenic processes influence flow through unsaturated tuff. Geochemical investigations will include the determination of the chemical composition of fluids and gases, as well as tracer experiments. Naturally occurring gases, CO_2 and radon (and perhaps other gases), will be monitored. These gases, and possibly artificial gas tracers, will be monitored in sealed intervals of the borehole as well as in drift sections adjacent to the borehole immediately after sealing off the drift. Relative humidity will be monitored in the same fashion. These field activities will provide information on gas movement in the near-drift zone. Monitoring in sealed intervals of boreholes will begin during the drift ventilation and will continue under nonventilated conditions. Carbon dioxide compositions in sealed intervals of the borehole will also be measured to assess the range of pH in pore waters, knowledge that is critical for evaluating the composition of potential seeps. Carbon dioxide and water isotopic analyses will also be performed to locate the source of CO_2 and water. Any collected water and dust accumulated on drift walls will be analyzed to determine its chemical composition, including stable and radioactive isotopes, which will help in evaluating water origin (e.g., liquid flow versus condensation).

   Moisture and gas dynamics around drifts could also be affected by the mountain "breathing" (i.e., air moving in and out of the mountain as a result of barometric pressure changes). To evaluate the processes involved in such "breathing," we will investigate whether advective gas fluxes caused by changes in atmospheric pressure dominate diffusive fluxes. Pressure changes affected by barometric fluctuations have been recorded at significant depth in the mountain. However, because of the low rock permeability, resulting advective fluxes for gases such as CO_2 may be small in comparison with those from gas concentration gradients (i.e., near-surface CO_2 concentrations are higher than those in the deep segments of the unsaturated zone, and high CO_2 concentrations are detected in groundwater). Therefore, both ambient pressure and gas composition will be monitored closely, both in the drift and sealed intervals, and these measurements will be used in conjunction with the results of existing permeability tests in the ECRB to quantify the magnitude and direction of ambient advective gas fluxes in the vicinity of the drift.

   To evaluate moisture dynamics within the tunnel under both ventilated and heated conditions, a new horizontal borehole will be designed as an analogue to a waste emplacement tunnel. This borehole will be subject to microclimates deemed similar to that of emplacement drifts, and dynamics within the borehole will be carefully monitored.

2. Numerical Modeling

   2-D or 3-D modeling will be performed to incorporate the results of field investigations and verify a conceptual model of flow and transport through fractured tuff in the near-drift zone. Vertically, the model domain will be on the order of 100 m or larger, with detailed discretization around the drift tunnel. The model will simulate the coupled processes of air and vapor dynamics, evaporation and condensation, and ambient percolation during ventilation and postclosure periods. The model will be calibrated using the moisture, temperature, and pressure-monitoring data collected from the ECRB tests. Using information gathered from this modeling effort, other previously developed seepage models will be enhanced to fully couple intradrift processes affecting seepage. These models will then be applied to study the impact of design decisions on seepage. The effects of geochemical and microbial processes will also be incorporated in these models. Results of the modeling could lay to rest the issue of the importance of cold traps to repository performance.

Schedule

Field investigations will be completed in five years. Numerical modeling investigations will continue iteratively with laboratory and field experiments.

Product

Annual letter progress-report to DOE and a series of journal articles, providing information to be used in design and maintenance of the emplacement drifts.

Level of Effort

The estimated resources for this work are:

	Year 1	**Year 2**	**Year 3**	**Year 4**	**Year 5**
Field Experiment	3 FTE	3 FTE	3 FTE	1 FTE	1 FTE
Numerical Modeling	2 FTE	2 FTE	2 FTE	--	--

The project will require purchase of equipment, construction, and drilling.

References

Salve, R., and C. M. Oldenburg, 2001.Water flow in a fault in altered nonwelded tuff. *Water Resources Research,* 37: 3043-3056.

Salve, R., J.S.Y. Wang, and C. Doughty, 2002. Liquid flow in unsaturated fractured welded tuffs: I. Field investigations. *Journal of Hydrology*, 256: 60-79.

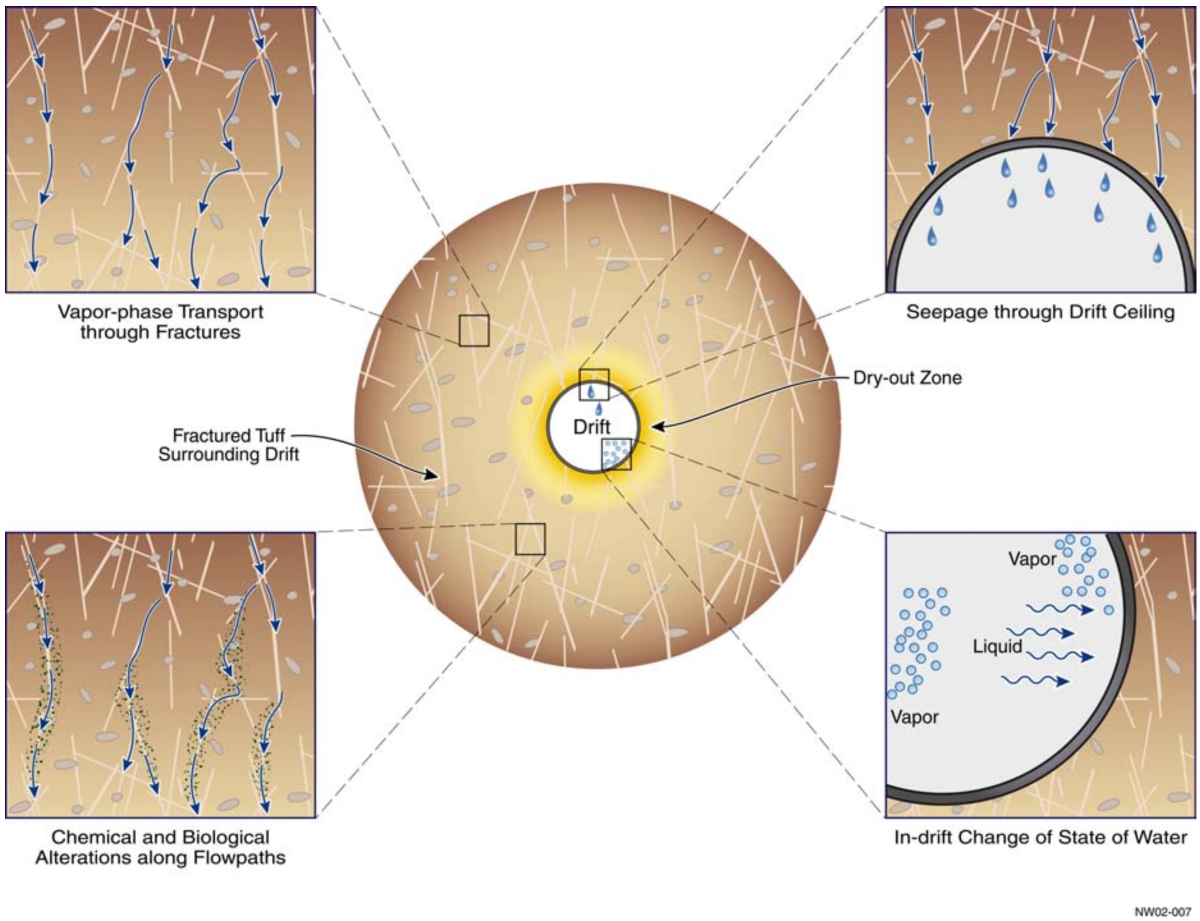

Figure F-1. Schematic of near-drift flow and transport processes affecting the drift microclimate

Figure F-2. Evidence of moisture in the nonventilated Cross Drift at Yucca Mountain: (left) moisture rivulets, (center) mold along tracks, and (right) rust and water drops on conveyor belt.

G. A Decision–Management Framework for the Design and Operation of the Preclosure Ventilation System at Yucca Mountain for Thermal Load Control

Focus Area: Unsaturated Zone
Contact: André Unger, AJAUnger@lbl.gov, (510) 495-2823
Collaboration: LBNL with the University of Waterloo, Canada

Statement of Problem

Forced ventilation of the waste drifts is needed as part of the preclosure ventilation system in order keep repository temperatures from exceeding a regulatory limit. This proposal will focus on developing a numerical model to predict the expected thermal load control behavior of the preclosure ventilation system and uncertainty in its behavior due to imperfect knowledge of formation properties. The thermal load controlling ventilation rate predicted by the model will be used to estimate the demand for electricity needed to operate the preclosure ventilation system. Uncertainty in the demand for electricity coupled with volatility in the price of electricity itself will expose the YMP to significant cost risk in operating the preclosure ventilation system. This proposal focuses on developing a decision-management framework to couple the demand for electricity forecasted by the ventilation model with a financial model to reduce the cost risk posed by the volatility in the price of electricity. The objective of this framework is to operate the pre–closure ventilation system at lowest cost by purchasing electricity on a futures market using financial option pricing models.

Background

Thermal load on the repository walls due to radiation from the waste packages will be controlled with enhanced vaporization of formation water by drawing formation gases into the waste drifts during forced ventilation. The interaction between ventilated air and formation gases was quantified on the basis of radon concentrations measured within the ESF (Unger et al., 2002). As part of thermal load control, the ventilation system will be operated at different rates to ensure that the exhausted air (and hence repository wall) temperatures do not exceed a regulatory limit. An increase in the operational capacity of the exhaust fans will cause a corresponding increase in suction, which will induce a proportional increase in the rate of ventilated air within the waste drift. This same increase in suction will also draw more formation gases into the waste drift, enhancing evaporation within (and hence cooling of) the TSw. The balance between the flow of ventilated air and formation gases (and hence the efficiency of the ventilation system) will be highly sensitive to uncertainty in the TSw fracture continuum permeability, in a manner identical to that indicated by the radon data. This uncertainty will have a direct impact on the efficiency of the ventilation system for thermal load control. The cost of operating the ventilation system for thermal load control is a function of the price of electricity multiplied by the demand for electricity needed to run the exhaust fans. This cost will be exposed to large uncertainty due to volatility in the price of electricity. The cost uncertainty is further compounded by uncertainty in properties of the TSw surrounding the waste drifts, and how these properties control the balance of formation gases and ventilated air in the waste drifts and hence the efficiency of the ventilation system for thermal load control. Given the need to ensure that repository temperatures do not exceed a regulatory limit, a decision-management framework is needed to design and operate the ventilation system to minimize costs, despite the uncertainties described above. As part of the decision-management framework, a method is described that will couple a ventilation model of a waste drift with an option-based financial model that can evaluate operational decisions regarding the pre-closure ventilation system. In particular, the ventilation model will be used to assess the mean and uncertainty in the demand for electricity needed to operate the exhaust fans to regulate the temperature of the repository. The option-based financial model will be used to evaluate the cost of purchasing a block of electricity at a fixed price to adequately supply the demands of the ventilation system over a fixed period of time at a future date.

The development of modern financial option pricing models began with the work of Black and Scholes (1973) and Merton (1973). Their modeling approaches have since been refined by academics and adopted by financial institutions around the world. Hull (1997) and Wilmott (1998) provide detailed reviews of the field of financial engineering including an in-depth analysis of many option-based financial products. Option-pricing models have begun to receive interest as a means to value projects with “real” assets (Dixit and Pindyck, 1994). In this case, “real options” are used to value managerial flexibility given volatility in market prices associated with goods to be delivered from the project. The value of managerial flexibility is analogous to purchasing insurance for protection against downside risk. In the context of this work, real options will be used to value managerial decisions regarding electricity purchases needed to operate the "real" asset which is the ventilation system.

Impact/Importance to the Yucca Mountain Project

The importance of this work will be to lower the total costs of operating the preclosure ventilation system for thermal load control. Furthermore, the proposed methodology will inherently account for uncertainty in the efficiency of the ventilation system due to heterogeneous formation properties, and how these would impact operational costs.

The pre-closure ventilation system will be operated for a minimum of 50 years. Preliminary calculations indicated that the air velocity within the waste drifts would need to be 10 m/s for thermal load control. Given 110 km of waste drifts, and assuming that the average length of a waste drift is 1 km with 0.5 km of inflow and outflow shafts, the ventilation system would need approximately 130 MWatt hrs of electricity if the exhaust fans operate at 20% efficiency. Assuming the annual average price of electricity is $30 per MWatt hr, the ventilation system will cost approximately $35 million per annum to operate. Clearly, it is in the best interests of the YMP to purchase this electricity in a cost-effective manner.

Objective

The objective of this work is to develop a decision-management framework for operating the preclosure ventilation system. This framework will couple a numerical model representing the efficiency of the ventilation system (and consequently the demand for electricity needed to operate the exhaust fans) for controlling thermal load in waste drifts with a financially based real option model to value alternative means of buying electricity to supply the ventilation system. The model will inherently account for uncertainty in the demand for electricity in the ventilation model due to uncertainty in formation properties controlling the mixing of ventilated air with formation gases, as well as volatility in the market price of electricity itself. The goal of this work is to enable the ventilation system to be operated at the lowest cost while ensuring that repository temperatures do not exceed a regulatory limit.

Workscope

The workscope will consist of four tasks.

1. Development and Calibration of a Ventilation Model

   Development of the ventilation model will largely follow prior work by Unger et al. (2002) where radon data were used to infer large-scale fracture continuum properties of the TSw. The basis for this strategy is to use permeability and porosity values obtained from calibration to the radon data, as well as to follow a model where the interaction between formation gases and ventilated air is well understood. This model will be extended by adding humidity and temperature data from the ESF in order to calibrate properties affecting the vaporization of water from the tuff matrix. Thermal properties of the TSw will be obtained from Tsang and Birkholzer (1999) and from other ongoing measurements in the underground drifts. This will enable the model to predict (forecast) the thermal load behavior of the ventilation system.

2. Evaluate Efficiency and Electricity Demand of Ventilation Model

   The efficiency of the ventilation model will be a function of how uncertainty in formation parameters affect the balance of formation gases and ventilation air in the waste drift for a prescribed ventilation rate. As the preclosure ventilation system is being simulated, model-calculated deviations between the repository wall temperatures and the regulatory limit, due to barometric fluctuations and variations in the suction induced by the exhaust fans, will be minimized using iTOUGH2 (Finsterle, 1999) by adjusting the ventilation rate. A conceptual example of how feedback from repository temperatures would affect the applied ventilation rate is shown in Figure G-1. In this case, as the repository temperature increases towards the regulatory limit, the ventilation rate is also increased. This pattern occurs until the repository temperature is reduced below the regulatory limit. At this point, the ventilation rate is reduced to conserve energy and the pattern reestablishes itself.

A relationship between ventilation rate (representing the speed at which the exhaust fans are being operated) and the demand for electricity will be assumed. The calibrated ventilation model will then be used to forecast the demand for electricity needed to control the thermal load within the waste drift over a specified period of time (such as a one-week interval). Furthermore, the uncertainty in this demand will be assessed due to uncertainty in barometric pressure conditions as well as TSw properties controlling the mixing of ventilated air with formation gases and hence the efficiency of the ventilation system. An example realization of the demand function is shown on Figure G-2a.

3. Development of Real Option Model

The objective of this task is to mathematically formulate and develop a numerical real option model to price the opportunity value of buying a block of electricity at a fixed wholesale cost to supply the demand of the ventilation system at a future date over a specified period of time. By purchasing electricity at a future date based upon the forecasted demand, the model will reduce the cost risk of operating the preclosure ventilation system given volatility in the price of electricity.

Many contracts could be valued to supply the electricity demand of the ventilation system including building a power plant dedicated to the YMP and selling the excess power into the regional grid. Assuming the YMP chooses to purchase all of its electricity from the spot market, the management-operator of the ventilation system may be able to negotiate the purchase of a block of electricity one month in advance to be supplied over a one week interval for a fixed rate which is slightly lower that the average weekly rate. An example realization of the price of electricity obtained from the CAISO Imbalance Energy Market from May 1st to 20th 2000 is shown in Figure G-2b. Given the highly volatile nature of the price of electricity, purchasing a block of electricity for a fixed rate which is slightly lower than the average weekly rate would significantly reduce the cost risk of operating the pre-closure ventilation system to the YMP.

The downside of this contract for the management operator is that they would be committed to purchasing the entire block of electricity even if it is not completely used. Furthermore, if the block of electricity is insufficient to supply the demands of the ventilation system, then they must purchase the shortfall on the spot market at higher and volatile rates. Clearly, it is in the management operator's interest to limit the lower bound on this payoff function, representing the (negative) cost of over– or under-supplying the amount of electricity needed to meet operational requirements. The impact of the lower boundary on the payoff function can be valued within an option-pricing framework where the underlying (and observable) stochastic variables are the price of electricity and the demand for electricity obtained from the physical model.

4. Decision-Management Framework

The objective of this task is to couple the ventilation model with the real option financial model and simulate the purchase of electricity to meet the forecasted demand of the preclosure ventilation system.

Schedule

Year 1: Tasks 1 and 2

Year 2: Tasks 3 and 4

Product

The deliverable upon completion of this project will be the mathematical framework and numerical models for evaluating the efficiency of the ventilation system for thermal load control, as well as the option value of purchasing a block of electricity to satisfy the operational demand of the ventilation system. An annual progress report to the DOE as well as journal publications will also be completed as part of this work.

Level of Effort

	Year 1	**Year 2**
Task 1	1.25 FTE	—
Task 2	1.0 FTE	—
Task 3	0.4 FTE	1.375 FTE
Task 4	—	1.5 FTE

References

Black, F. and M. Scholes, 1973. The pricing of options and corporate liabilities., *Journal of Political Economy*, 81, 637–659.

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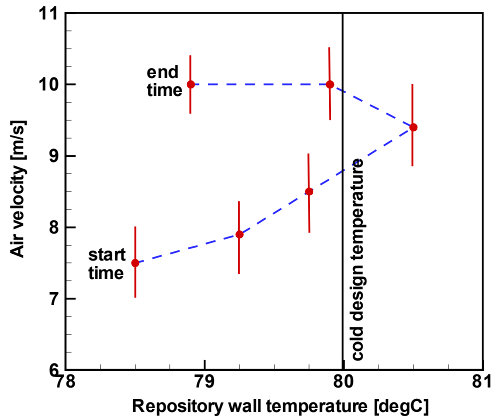

Figure G-1. Control–feedback loop between the air velocity in a waste drift and the repository wall temperature

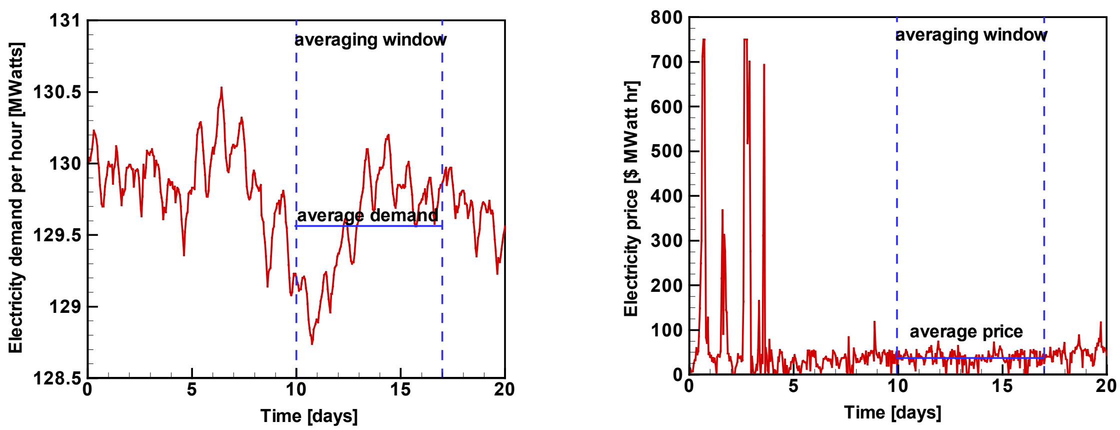

Figure G-2. (a) Forecasted electricity demand of the pre–closure ventilation system and (b) the spot price of electricity obtained from the CAISO Imbalance Energy Market from May 1 to 20, 2000

H. Evaluation of the Drift Shadow Model and Model Extensions

Focus Areas: Unsaturated Zone, Coupled Processes, Natural Analogues
Contact: Jim Houseworth, JEHouseworth@lbl.gov, (702) 295-7611
Collaboration: LBNL

Statement of Problem

The drift shadow model of radionuclide transport near waste emplacement drifts is concerned with the transport of radionuclides released from drifts that experience no or significantly reduced drift seepage. In the previous transport models used for total system performance assessment (TSPA), fracture flow beneath waste emplacement drifts was assumed to be unaffected by the presence of the drift. Radionuclides released from waste emplacement drifts were assumed to preferentially enter the undisturbed flow in the fractures. However, the current seepage models used for performance assessment indicate that not all drifts will have seepage. Furthermore, models for the flow patterns around drifts without seepage indicate the presence of a zone of greatly reduced flow with nearly stagnant water immediately below the drift (see Figure H-1). In the absence of significant water seepage into the drift, radionuclide transport from the drift into the rock is expected to occur by means of molecular diffusion through the rock matrix. It is expected that long-term molecular diffusion will involve predominantly the low-permeability matrix, because about 99.9% of the available water is in the rock matrix. However, experimental investigations of the shadow zone problem are currently limited or unavailable.

Impact/Importance to the Yucca Mountain Project

Theoretical models for flow and transport in a homogeneous dual continuum indicate that a drift shadow will exist beneath a drift, with the extent and magnitude of the shadow being larger in the fracture continuum than the matrix continuum. Initial analyses performed for Supplemental Science and Performance Analyses (SSPA) were carried out for a two-dimensional, drift-scale model that extended 15 m above a potential waste emplacement drift to 45 m below the drift. This analysis indicates that transport of a non-sorbing radionuclide through 45 m of the host rock, given initial release to the rock matrix, will require thousands of years as compared with about one year if initially released to undisturbed (background) fracture flow. Figure H-2 shows breakthrough curves for a non-sorbing radionuclide (e.g. ^{99}Tc) under two distinct release scenarios: (1) release from a non-seeping drift to rock matrix, and (2) release from a seeping drift to undisturbed fracture flow, for a depth of 45 m beneath the potential waste emplacement drift within a single host-rock unit (TSw lower nonlithophysal unit). The significant increase in the breakthrough time in the case of simulating the drift shadow zone clearly indicates the importance of taking into account the shadow zone for modeling radionuclide transport that originates from drifts without seepage.

Furthermore, it is important to include in the analysis of the flow and transport processes the effects of thermal dryout. The dryout around drifts is expected to prevent radionuclide transport until re-wetting occurs below the drifts. Existing drift-scale thermal-hydrologic models indicate that for the high-temperature operating mode considered in TSPA-SR and SSPA the area beneath the drifts will remain dry for 2,500 to 3,000 years (Figure H-3). Including the effects of dryout, the estimated average travel time from the potential repository to the water table for a non-sorbing radionuclide released from a drift without seepage is on the order of 10,000 years or more under present-day climate and 6,000 years or more for a much wetter, future climate.

Given a regulatory period of 10,000 years, these significant delays in the breakthrough time for potential radionuclide migration must be taken into account in the repository performance analysis. Accurately representing these processes in the TSPA may show that the performance of the natural system alone meets, or nearly meets, regulatory dose requirements.

Thus, it is important to provide physical evidence of the existence of the drift shadow and address questions concerning the applicability of the drift shadow model to heterogeneous fractured rock at Yucca Mountain, including the effects of thermal dryout on radionuclide transport beneath waste emplacement drifts. This would allow a more accurate and detailed implementation of the drift shadow concept into TSPA.

Objectives

Obtain data to be used for developing and evaluating the drift shadow model. Investigate the effects of rock heterogeneity and thermal-hydrologic processes, particularly thermal dryout, on transport near waste emplacement drifts.

Workscope

The workscope is divided into five tasks:

1. Field testing of the drift shadow concept in fractured rock

   A preliminary test concept is to inject water over a small drift, approximately 2 m in diameter, and the water pattern distribution, and collect the water, if any, in a slot below the opening. Potential test locations under consideration are Alcoves 5 and 6 and Niche 5. A dry tracer would be added to the bottom of the drift. The collected water would be analyzed for tracer and the flow geometry in the slot would also be monitored. Boreholes below the drift would be monitored using electrical resistivity probes to determine wetting front arrivals. Drill-back in the test zone and/or post-test mine-back would identify the extent of tracer migration. The field test would demonstrate the presence or absence of a drift shadow zone, quantify radionuclide transport processes and seepage-diffusion interactions in repository host rocks, and measure flow and transport parameter changes below and around the drift. Test modeling would also be performed to evaluate the ability of the current conceptual model to represent field measurements.

2. Natural and/or anthopogenic analogue studies of the drift shadow concept in fractured rock

   Analogue studies in natural caves or old mine tunnels would be used to provide qualitative information on the behavior of flow and transport in the vicinity of an underground opening in unsaturated, fractured rock that occurs under natural conditions over long time periods. Sites under consideration include old mines in the vicinity of the Nevada Test Site, a tunnel at Apache Leap, Arizona, and a gypsum cave near Carlsbad, New Mexico. The studies would focus on identification of geochemical/isotopic compositional variability below the openings as compared to locations not sheltered by the opening. These studies complement the field tests described in task 1, which would need to be conducted over a time that is short compared to the 10,000 year regulatory period and at much higher flow rates than under natural conditions. (See also proposals O.1, O.3, and O.4.)

3. Relation between secondary minerals observed in lithophysal cavities at Yucca Mountain and the drift shadow

   Lithophysal cavities range in size from a centimeter to meters. The results of field experiments and modeling suggest that openings of this size should divert seepage. However, many lithophysal cavities have secondary mineral deposits originating from water flow. A possible resolution to this inconsistency is the possibility that water flows into the lithophysal cavity from below, as was observed during tracer injection tests at Niche 5. If the seepage and drift shadow models are correct, lithophysal cavities, like all macroscopic underground openings, should have a zone of very low flow below the cavities. Water films may be able to enter the cavities from all sides. However, sufficient concentration of dissolved solids, resulting from evaporation into the cavity air, may only be able to develop at the bottom of the cavity caused by the diffusion-limited mass transport on the lower side of the cavity. Reactive transport models will be used to investigate the potential relationship between the secondary minerals observed in lithophysal cavities and the existence of the drift shadow.

4. Analyses of drift shadow behavior for heterogeneous rock for steady, ambient flow conditions

   The initial drift shadow calculations performed for SSPA did not include the effects of heterogeneity. However, subsequent analyses have shown that if transport is initiated in the matrix, subsequent transport behavior is relatively insensitive to the presence or absence of fracture flow for low fracture saturation.

This result suggests that transport behavior is expected to be insensitive to the degree of heterogeneity of the fracture continuum. The study will consider transport behavior for a range of spatially correlated heterogeneous properties for the fracture and matrix continua.

5. Analyses of transport near waste emplacement drifts, accounting for the effects of waste heat

   These analyses would be used to investigate the effects of thermal dryout and re-wetting behavior on the potential release and transport of radionuclides from a waste emplacement drift. After initial investigations for homogeneous rock conditions, the analyses would be extended to include heterogeneous conditions. The studies would include both drifts with and without seepage. This task will result in developing a practical means of representing thermal-hydrologic effects on near-drift transport in TSPA.

Schedule

The schedule is given below by workscope area.

1. Field test construction and pre-test modeling: Year 1

   Field testing data collection: Years 2 and 3

   Sample analyses and post-test modeling of field data: Years 3 and 4
2. Analogue modeling and site selection: Year 1

   Analogue site data collection and sample analyses: Years 2 and 3

   Continued sample analyses and assessment of analogue data: Years 3 and 4
3. Analyses using two-phase, reactive transport model: Years 2 and 3
4. Analyses of steady-flow transport behavior in the drift shadow for heterogeneous rock conditions: First half of Year 2
5. Analyses of thermal-hydrologic effects on transport in homogeneous fractured rock: First half of Year 2

   Analyses of thermal-hydrologic effects on transport in heterogeneous fractured rock: Last half of Year 2

   Development of methods for implementation in TSPA: First half of Year 2

Product

The results of each of the workscope tasks will be published in peer-reviewed journals. Internal reports describing the scientific findings as well as proposed methods for implementation of these findings in TSPA will be produced. Annual progress reports will be prepared for DOE.

Level of Effort

The estimated resources for this work are given by workscope area. Construction, test equipment, sampling, and sample analyses will also be required.

	Year 1	**Year 2**	**Year 3**	**Year 4**
Task1	2 FTE	2 FTE	2 FTE	2 FTE
Task 2	1.5 FTE	2 FTE	2 FTE	2 FTE
Task 3	—	0.5 FTE	1 FTE	—
Task 4	—	0.5 FTE	—	—
Task 5	—	1 FTE	1 FTE	—

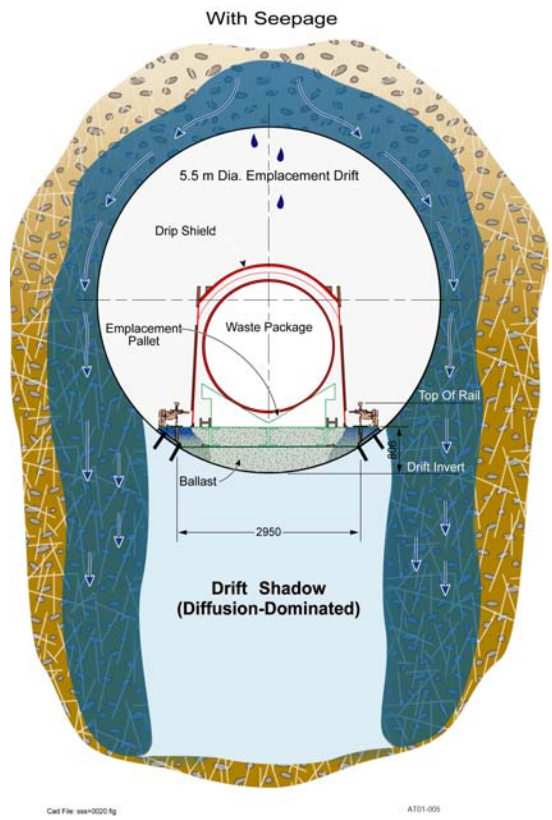

Figure H-1. Conceptual diagram of the drift shadow

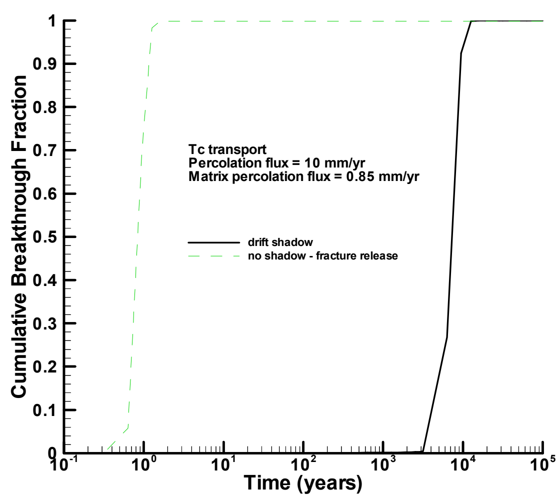

Figure H-2. Tc breakthrough at 45 m below potential waste emplacement drift

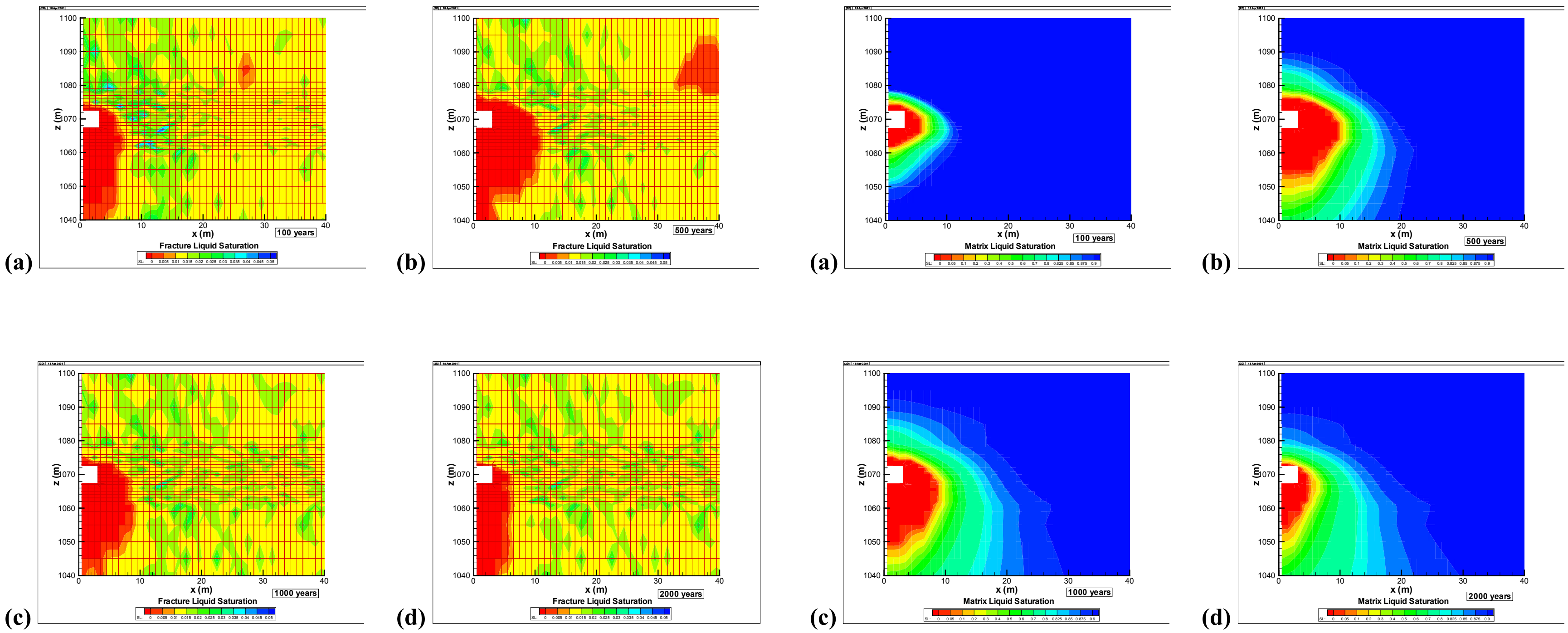

Figure H-3. The effects of dryout on liquid saturation distributions in the fracture and matrix continua for the higher-temperature operating mode used in the SSPA (Note: the greater spatial extent and longer duration of dryout beneath the waste emplacement drift as compared with the top. This asymmetric pattern is a result of drift shadow effects on re-wetting.)

I. Colloid and Nanoparticle Transport in Yucca Mountain Unsaturated Zone Rocks and Fractures

Focus Area: Unsaturated Zone Transport
Contact: Jiamin Wan, JMWan@lbl.gov, (510) 486-6004
Collaboration: LBNL

Statement of Problem

It has become recognized that transport of highly sorptive radionuclides is very limited in solution, and the most efficient mode of radionuclide migration is through association with mobile colloids (e.g., Penrose et al., 1990; Kersting et al., 1999). Large uncertainties in the anticipated degree of colloid-facilitated radionuclide transport from the repository exist because of significant knowledge gaps.

Knowledge Gaps on Colloids in the Yucca Mountain Site: Colloid transport has been an important research area since the beginning of the Yucca Mountain Project. Research has been focused on interactions between radionuclides and colloids (K_d measurements), colloid transport in the high-permeability zone far away from the repository (e.g. vitric Calico Hills tuffs), and under saturated conditions. Much useful information has been gained in the past decade and key issues are being addressed, such as waste form degradation and colloid formation, and colloid concentrations. However, a few highly relevant processes have not been explicitly addressed by previously YMP-funded colloid studies. Figure I-1 shows the source zone of radionuclide-associated colloids, directly under the waste package. If the drift shadow zone concept holds, there will be no water in the shadow zone fractures, and colloids cannot escape through dry fractures. The only pathway will be through the TSw tuff matrix. Can colloids diffuse into the tuff matrix? Can colloids migrate through the tuff matrix and if so, how far? On the other hand, if the shadow zone is not as dry as expected, the fractures will still probably not be saturated, and film flow may be one of the dominant mechanisms for unsaturated flow underneath the repository. The extent to which colloids will move under negative matric potentials during film flow on fracture surfaces is not yet understood.

Knowledge Gaps in Fundamental Science: Current understanding of colloid transport is largely based on filtration theory developed earlier in the area of chemical engineering for wastewater treatment. Filtration theory can be successfully applied to colloid transport in water-saturated subsurface porous media, but is not directly applicable to transport through the unsaturated zone (UZ). The basic physics and chemistry unique to UZ zone colloid transport is a consequence of the existence of the second immiscible fluid phase, air, which results in: (1) saturation dependent flow, and (2) an additional interface, the air-water interface (Figure I-2). Understanding UZ zone colloid transport largely depends on our knowledge of flow in the UZ zone, and knowledge of constraints imposed by the air-water and water-solid interfaces on colloid mobility. Film flow has been identified as an important mechanism of water flow along unsaturated rock fractures (Tokunaga and Wan, 1997, 2001a, b; Tokunaga et al. 2000). However, thin water films can retard colloid transport, and a film-straining model was introduced for unsaturated colloid transport (Wan and Tokunaga, 1997), which describes the fundamental difference between colloid transport in partially saturated versus saturated media. Evidence for sorption of certain colloids at air-water interfaces in subsurface environments was provided (Wan and Wilson, 1994a, b; Wan et al. 1994). Recently, the first method for measuring partitioning of colloids at air-water interfaces was developed (Wan and Tokunaga, 1998), and partition coefficients of common clays were determined (Wan and Tokunaga, 2002). These previous studies revealed the processes important in colloid transport/retardation in unsaturated subsurface environments. However, none of these aforementioned new developments on unsaturated colloid transport has been applied to the Yucca Mountain fractured tuff rock system.

Knowledge Gaps in Nanoparticles: The earth science community has recently identified environmental nanoscience as an emerging field. The National Science Foundation and the DOE Basic Energy Science and Environmental Management have recently developed specific research programs on Nanoscience in the Environment. Although nanoparticles (1–100 nm) are within the colloidal domain (1–1,000 nm), particles in this very small size range are often not studied because of limitations in techniques and instrumentation. Due to their very small sizes, nanoparticles are highly reactive and are assumed to have high mobility in the subsurface. One of the most often asked questions by the public and larger scientific community is what the impact is of nanoparticles on radionuclide transport in the subsurface. Present knowledge indicates little quantitative information specifically addressing size-dependent transport in the subsurface, but much speculation. The YMP needs to act quickly to address the issue of possibly enhanced actinide transport by nanoparticles. A realistic, site-specific understanding of nanoparticle transport in Yucca Mountain needs to be obtained.

Impact/Importance to the Yucca Mountain Project

- Dispersed nanoparticles are expected to be unstable (they will form aggregates/flocculates) under Yucca Mountain geochemistry conditions.
- Colloid transport within the tuff matrix is expected to be ineffective due to extremely small pore sizes.
- The unsaturated condition provides tremendous resistance for colloid migration along fracture surfaces (film straining).
- Completion of this proposed research will substantially reduce uncertainties associated with colloid- and nanoparticle-facilitated radionuclide transport from the repository.

Objectives

The overall objective of this research is to provide an experimentally tested, site-specific conceptual model, and a predictive model for colloid transport through unsaturated fractures and matrix tuffs of Yucca Mountain. The detailed objectives are:

- Identifying the importance of nanoparticles on enhancing radionuclide transport in Yucca Mountain. Whether or not dispersed nanoparticles are stable under the chemistry conditions of Yucca Mountain will be tested. The results will establish the lower boundary for relevant colloid sizes for potential transport at Yucca Mountain.
- Testing whether or not colloids can diffuse through tuff rock matrix. If yes, the practical ranges for filtration coefficients and their primary controls will be determined. If no, colloid transport should be further evaluated only within fractures.
- Quantifying colloid transport on fracture surfaces during steady unsaturated flow conditions to obtain the relations of matric (capillary) potential, colloid type and size, and colloid film straining (retardation rate).
- Developing a site-specific, predictive model for colloid transport through Yucca Mountain, by incorporating quantitative information and conceptual models from laboratory experiments into the TOUGH2 colloid module.
- Applying the model to Yucca Mountain to predict the long-term significance (or insignificance) of colloid-enhanced radionuclide transport.

Workscope

1. Stability of nanoparticles

   Based on current studies, nanoparticles have a strong tendency to flocculate, form aggregates, and become less mobile (Figure I-3). The stability of nanoparticles will be studied under Yucca Mountain geochemical conditions. The effective size range of colloids will be identified under chemical conditions relevant to the Yucca Mountain site. This defined size range will be used in the rest of the transport experiments. In order to test nanoparticle stability, uranium and iron-oxide nanoparticles will be synthesized. The nano-sized fraction of clay and silica particles will also be used.

2. Colloid transport/diffusion into rock matrix

   It is expected that colloids will be efficiently filtered (retarded) by the TSw tuff matrix. Whether, or to what extent, colloids can be transported though the tuff matrix will be tested. These tests will be done by contacting colloidal suspensions in tracer (KBr or LiBr) solutions with repository horizon tuff rocks. Gold and uranium colloids (a few to 100 nm) will be used, because they are easily detected within the matrix using the synchrotron x-ray fluorescence microprobe. The dependence of colloid transport on colloid sizes will be determined. Very limited transport distances are anticipated due to efficient filtration within the very fine tuff matrix pores. The x-ray microprobe will be able to map even very shallow penetration (e.g., 10 μm). These results will determine whether on not colloid transport through the tuff matrix needs to be considered.

3. Colloid transport on fracture surfaces during steady, unsaturated flow

   Figure I-4 shows our conceptual model of film straining of colloids on fracture surfaces. In the experiments, film flow will be established over a range of matric potentials (-15 to -0.01 kPa). Laboratory methods similar to those described in Tokunaga and Wan (1997), and Wan and Tokunaga (1998) will be used. These tests will be done on single, unsaturated fractures. Additional steady film flow colloid transport experiments will be done on the cubic meter block. The dependence of colloid transport on matric (capillary) potential, colloid type, and size will be quantified through these experiments. Most laboratory colloid transport studies use polystyrene latex microsphere as model colloids because they have well characterized properties and are easy to handle. However, the colloids most likely to associate with radionunclides are those formed during waste form corrosion. These site-specific colloids will be used in this task.

4. Developing a predictive model

   The quantitative information and conceptual model from laboratory experiments will be incorporated into TOUGH2. A site-specific, predictive model for colloid transport through Yucca Mountain will be developed.

4. Applying the model

   The model will be applied to the YM repository to predict the long-term significance of colloid-enhanced radionuclide transport.

Schedule

This work is proposed as a 3-year research project.

Task 1– Nanoparticle stability: Year 1.

Task 2– Colloid transport through matrix diffusion: Year 1, Year 2.

Task 3– Colloid transport in unsaturated rock fracture surface: Year 2, Year 3.

Task 4– Developing a predictive model: Year 1, Year 2, Year 3.

Task 5– Applying the model to YM: Year 3.

Product

Annual progress reports will be prepared for DOE.

The results of each of the workscope tasks will be published in peer-reviewed journals.

Level of Effort

The laboratory experiments are very technically challenging, labor-intensive, and provide the foundation for defensible predictions of colloid transport. Therefore, we propose 2 FTE for the lab part and 1 FTE for the modeling part each year. We also request some support for routine lab supplies and external sample analyses (such as electron microscope fees, at $60-90/h).

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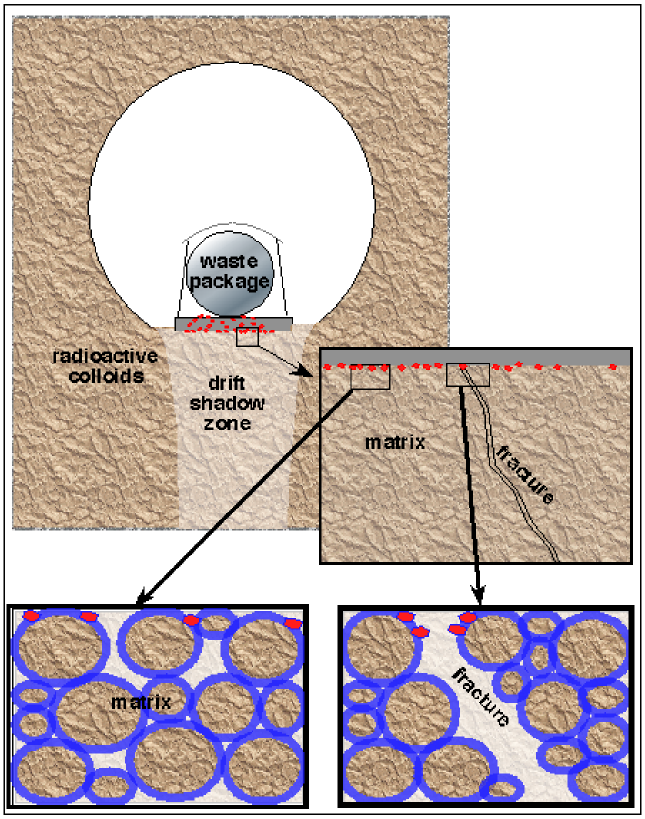

Figure I-1. Conceptual model of colloid transport in the drift shadow zone

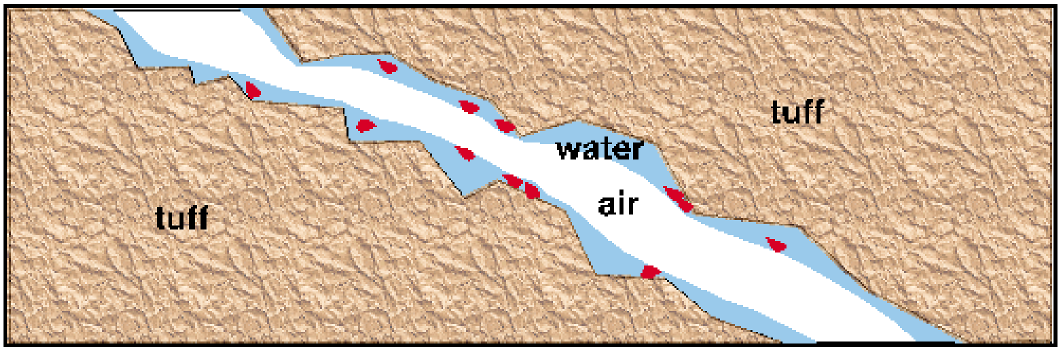

Figure I-2. Conceptual model of colloid transport in water films along the fracture surfaces

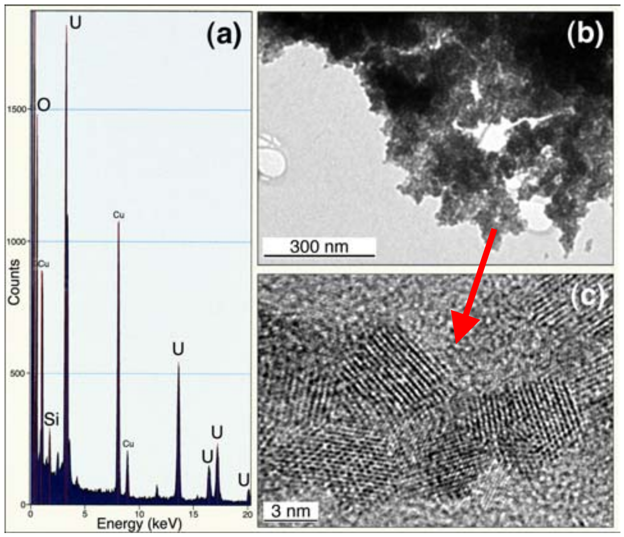

Figure I-3. TEM analyses of laboratory synthesized U(VI) nanoparticles. The nanoparticles formed aggregates when suspended in a solution of pH 7.8, and 1.0 mM NaCl. (Wan et al. 2002, unpublished)

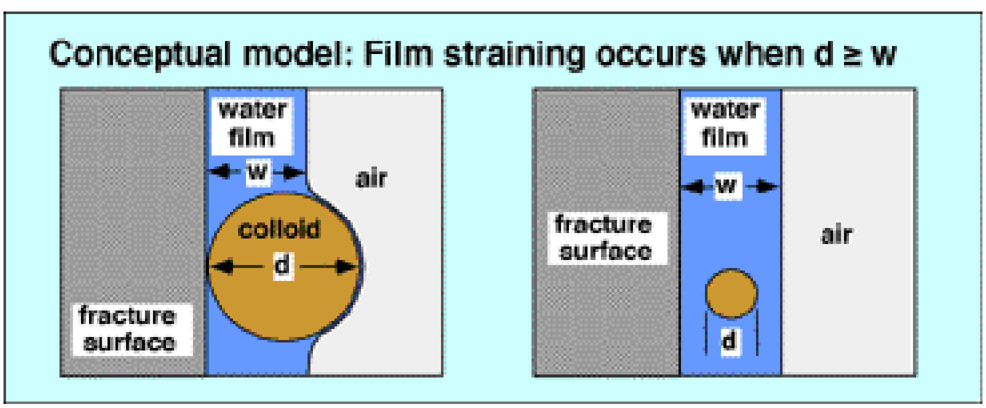

Figure I-4. Conceptual model of film straining of colloids on a fracture surface

J. Effects of Diffusion and Sorption on Radionuclide Transport in the Unsaturated Zone of Yucca Mountain: An Integrated Experimental and Modeling Study

Focus Area: Unsaturated Zone
Contact: Qinhong (Max) Hu, H_Qu@lbl.gov, (510) 495-2338
Collaboration: LBNL

Statement of Problem

In the unsaturated zone (UZ) at Yucca Mountain, water flows predominantly through the interconnected fracture network, with some water imbibing into the neighboring rock matrix. The size of rock matrix (i.e., fracture spacing) between flowing fractures could be large (e.g., in tens of centimeters). Radionuclide exchange occurs between the fractures and rock matrix through advection and diffusion. Many aqueous radionuclides will also sorb to the rock due to chemical interactions. All these interacting processes (imbibition, diffusion, and sorption) tend to retard radionuclide transport. However, these interacting transport processes are not well understood and their associated parameters have not been sufficiently quantified for transport through unsaturated fractured tuff at Yucca Mountain, as much of previous transport work utilized crushed (instead of intact) rock. Furthermore, how these processes and complex flow patterns interact in fracture networks within the UZ is unclear.

Background

In studies of radionuclide transport and retardation for Yucca Mountain, the effective sorption distribution coefficient (K_d) approach has been employed to quantify the extent of radionuclide-rock interactions. Experimentally determined sorption values are predominantly derived from laboratory batch experiments using crushed tuff (with a sample size of 75–500 μm) under water-saturated conditions (with a solution/solid ratio of 20) (Figure J-1a). However, it is problematic to use batch-sorption results to describe radionuclide transport through fractured rock in the UZ, because: (1) saturated and well-mixed conditions can overestimate radionuclide sorption in comparison with the UZ characteristic of fast flow and preferential flowpaths with a limited area for radionuclide-rock interaction; (2) crushing of whole rock could create new contact surfaces as well as increase radionuclide accessibility to sites that may not contribute to sorption if rocks were intact; and (3) for weakly sorbing radionuclides, batch tests can yield negative (i.e., exclusion instead of sorption) values with large variability. Therefore, a new approach is proposed, called the unsaturated transport-sorption approach, to generating sorption values, using large-sized (centimeters to several tens of centimeters) intact rock under unsaturated transport conditions (Figure J-1b). This approach will overcome the problems of batch-sorption experiments and lead to a realistic quantification of retardation in the UZ and increased confidence in the site-scale transport modeling. Matrix diffusion can significantly slow the advance of radionuclides undergoing advective fast transport through fractures. However, two issues need to be addressed regarding this important process in the UZ at Yucca Mountain.

1. Direct evidence of matrix diffusion in the UZ has not been fully established, mainly because of the lack of diffusion experiments in unsaturated fractured rock. Sampling protocol for geochemical studies commonly involves extracting pore water from the rock matrix, and this homogenizes the diffusion concentration profiles: the measurable chemical/isotopic tracer concentration is limited to the centimeter range from the fracture-matrix interface. In this proposed work, a microscale profiling technique will be used (therefore, experiments conducted over a reasonably short duration) to directly examine diffusive distribution of chemicals in the rock matrix from the fracture-matrix interface.

2. Assessment of matrix diffusion at Yucca Mountain is mainly (if not solely) based on the diffusion measurements in six pieces of devitrified tuff under saturated conditions, as reported in CRWMS M&O (2000). Nevertheless, the extent of diffusion is not necessarily linearly related to water saturation, as the current diffusion model assumes. This linear relationship may only hold at relatively high water saturation. At low water saturation, many of the pores can be separated by thin water films, through which diffusion is evidently very slow; thus, linear relationships will greatly overestimate the extent of diffusion. A two-part diffusion model with respect to water saturation needs to be developed and

implemented into UZ transport modeling. New conceptual models will be explored, including those based on fractals and pore networks. Findings from this unsaturated diffusion work will also have direct application to diffusive process characterization in the drift shadow zone, as well as to the invert in the Engineered Barrier System (Figure J-1).

Heterogeneities at different scales can have dramatic effects on flow and transport between fractures and the matrix. Note that fracture-matrix interaction is mainly determined by flow patterns in an unsaturated fracture network (Liu et al., 1998). While the proposed experimental work is focused on relatively small scales, discrete modeling work will be performed to "bridge" small-scale findings to large-scale behavior. Recently, Liu et al. (2002) used a fracture-network model and found that average spacing between active flow paths in the UZ of Yucca Mountain decreased with depth, owing to large-scale heterogeneities. This has important implications for how fracture-matrix interaction affects radionuclide transport. Since this mechanism has not been considered in current models, an improved understanding could significantly reduce uncertainties in the UZ flow and transport models for total system performance assessment (TSPA).

Impact/Importance to the Yucca Mountain Project

Given dramatically different velocities for water flow and radionuclide transport through fractures and matrix, an improved understanding of matrix diffusion and sorption at different scales, and more reliable quantification of the related parameters, will significantly reduce the uncertainties involved in the TSPA (OECD and IAEA, 2002). This work has the potential for demonstrating increased performance of the natural barrier with a combination of carefully designed laboratory experiments and numerical simulations of matrix diffusion and sorption processes at different scales. These processes are key mechanisms for retarding radionuclide transport in the UZ of Yucca Mountain. Furthermore, verification of the existing sorption parameters for intact rock versus crushed tuff is essential for increasing the credibility of radionuclide transport models used in TSPA.

Objectives

The specific objectives of this proposal are to:

1. Obtain representative sorption values for radionuclides using intact tuff samples (scales up to tens of centimeters) and validate the applicability of sorption values measured using crushed tuff.

2. Investigate and quantify unsaturated diffusion processes for different types of tuff at Yucca Mountain and explore new conceptual models for describing matrix diffusion.

3. Better understand and quantify the interacting imbibition, matrix diffusion, and sorption processes in unsaturated tuff.

4. Examine the interaction between these processes and complex flow patterns in fracture networks, thus reducing the uncertainty of the site-scale UZ transport model.

Workscope

1. Rock Sample Preparation

   Three major tuff types (i.e., zeolitic, vitric, and devitrified) at Yucca Mountain will be collected, characterized, and used. Part of the samples will be crushed into several-sized fractions. Characterization will include the measurements of porosity, permeability, water retention curve, surface area, and pore size distribution.

2. Unsaturated Transport-Sorption Experiments

   Tests will be conducted by placing one end of a sample in contact with water containing chemical mixtures. Imbibition will transport chemical tracers farther away from the tracer source. Sorbing tracers will be subjected to retardation, which leads to delayed transport (Figure J-1b). Such an approach enables investigation of the chemicals with very small (yet nonzero) sorption, as shown in Hu et al.

(2002). The tests will be conducted with different tuff types and sizes, as well as initial water saturations, to encompass the expected range of conditions (e.g., relatively dry conditions in the drift shadow zone) in the UZ. The following techniques will be used to examine chemical concentration as a function of distance in the sample.

- Rock samples (with sizes of a few centimeters) will be profiled for chemical distribution using laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS), a recently developed technique at LBNL with a spatial resolution in the range of microns.
- For larger samples (centimeters to tens of centimeters), a drilling technique described in Hu et al. (2002) will be used for sampling and drilled rock at discrete intervals (e.g., 1 mm) extracted for subsequent chemical concentration measurements.
- The use of x-ray computed tomography (CT) scanning will be explored to monitor the movement of fluids in real time. The dual-energy mode of CT allows water and tracer movement to be simultaneously monitored, thus generating instant retardation values *in situ* (both spatially and temporally). The sample size applicable for CT scanning could be up to 10 cm in diameter and 100 cm in length. Such sample sizes have not been attempted in any sorption investigation.

A mathematical model will be developed to describe transient transport-sorption processes and obtain sorption values. An inverse method developed for estimating hydraulic parameters (Pan and Wu, 1998) will be extended to this transport work. Conventional batch-sorption and saturated-column-transport experiments will also be carried out, using crushed tuff (with different size fractions). The results obtained will provide a direct comparison to these of intact rock used in the transport-sorption experiments.

3. Unsaturated Diffusion Experiments

Diffusion measurements will be conducted for different types of tuff under both saturated and unsaturated conditions by placing a rock sample laced with a mixture of tracer (i.e., the source rock) in contact with another sample without tracers (i.e., the sink rock). The initial condition is achieved by vacuum-saturating the samples with or without tracers. Samples for unsaturated diffusion tests are further prepared by equilibrating them separately within a specific relative humidity chamber to remove any potential nondiffusive processes (e.g., advective flow from different capillarity). Then, the diffusion tests are initiated by contacting these samples. After a certain diffusion duration, the LA-ICP-MS profiling technique will be used to determine tracer distribution, from which the diffusion coefficient will be obtained. Such unsaturated diffusion tests will be conducted at several water saturations controlled by different saturated salt solutions.

Matrix diffusion in transport modeling is conventionally described as a Gaussian process. If relatively poor connections between matrix pores (pore-scale heterogeneity) exist, this conventional approach is not adequate. Various tuffs at Yucca Mountain will be tested for their pore connectivity, according to the approach established at LBNL. If needed, a new model that treats matrix diffusion as a Levy process will be developed. The Levy process is a generalization of the Gaussian process and has been used for dealing with flow and transport in extremely heterogeneous systems.

4. Transport Involving Single Fracture-Matrix Interaction

A test design employing a single artificial fracture with adjacent tuff matrix will be constructed to directly investigate the interacting imbibition, diffusion, and sorption processes. A liquid containing tracers will be injected on the top, with the effluent monitored at the bottom. At the end of the test, tracer distribution from the fracture face into the matrix will be mapped, using the LA-ICP-MS profiling technique. Different experimental variables (e.g., liquid flux, initial tuff saturation, fracture aperture, and episodic flow events) will be examined. A mixture of tracer chemicals will be employed to investigate these interacting processes. For example, use of several nonsorbing tracers with differing diffusivity will help to directly evaluate if and when matrix diffusion is important, and use of different tracers during each episodic flow event will examine the episodicity effect on fracture-matrix interaction. Models will be developed and experimental results predicted based on sorption and diffusion data obtained from tasks above.

5. Transport in a Cubic-Meter Block

   This work will be conducted in conjunction with Proposal M, titled "Thermal-Chemical and Thermal-Mechanical Effects on Fracture and Matrix Properties". Tracer tests will be carried out in a cubic-meter tuff block that involves multiple fractures. Experimental design and result interpretation are similar to those described in the single fracture transport test.

6. Large-Scale Fracture Network Modeling for Transport

   In addition to single fracture-matrix modeling activities used for interpreting experimental observations, large-scale (on the order of 100 m), multidimensional, fracture-network models (including matrix) will be developed to "bridge" small-scale findings to large-scale radionuclide transport processes. The procedure to construct fracture networks described by Liu et al. (2002) will be followed. Simulations will be performed for fracture networks corresponding to a single geologic unit and several adjacent units to explore the effects of heterogeneity at different scales. Fracture-network modeling results will also be compared with results from the continuum-approach-based models to examine whether fracture-matrix interaction mechanisms are correctly captured by the continuum models used for TSPA. If needed, new continuum modeling approaches based on experimental observations and fracture-network modeling results will be developed.

Schedule

This proposed work could be completed in three years. Activities in the first two quarters include sample collection, test design, equipment setup, and pre-test modeling analyses. The tests are initiated at the end of the second quarter and last for about nine quarters. Syntheses of data, development of models (unsaturated core transport-sorption, unsaturated matrix diffusion, single fracture-matrix, cubic-meter block, and fracture networks), and report preparation will be carried out simultaneously with the tests. The last quarter will be devoted to final report and deliverable preparation.

Product

Results of this proposed work will be documented in research reports, an annual progress report to DOE on results of work to date, and will be submitted for publication in peer-reviewed journals (with more than three publications expected).

Level of Effort

Two FTEs per year for three years are needed to complete this proposed work.

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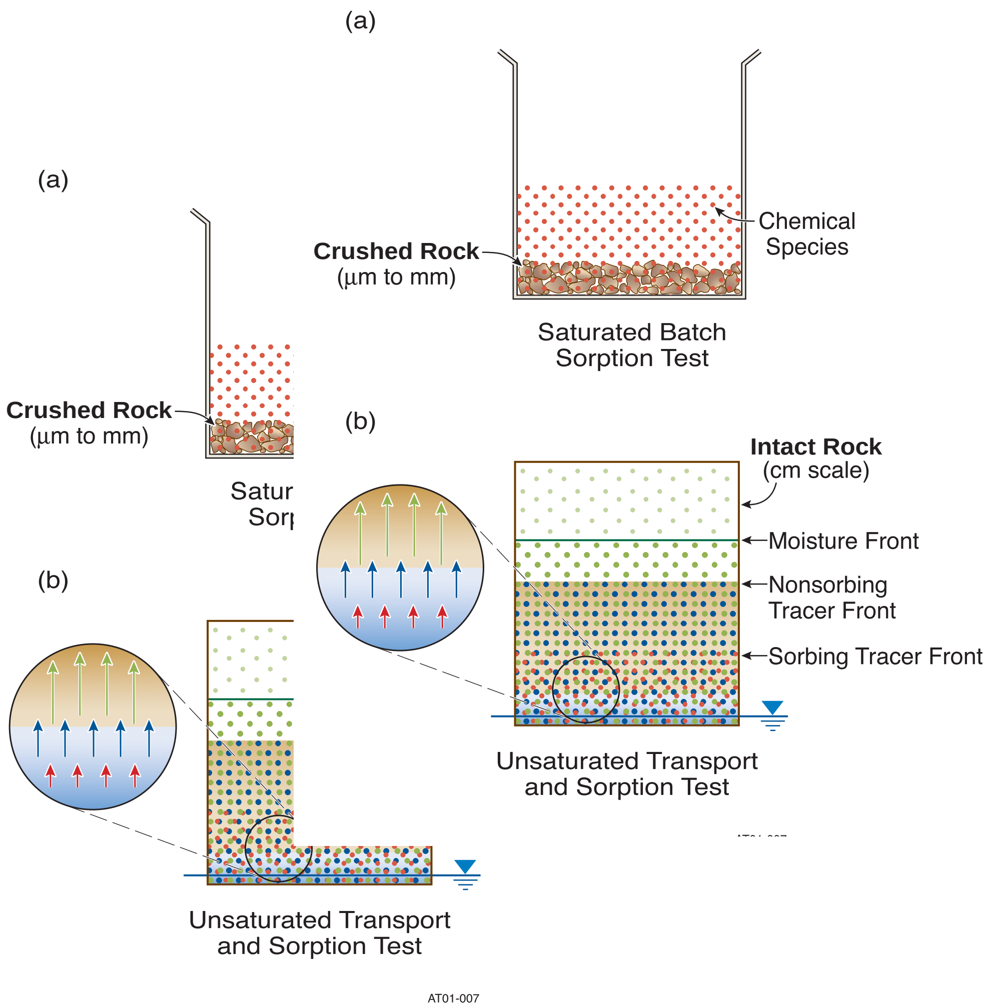

Figure J-1. Schematic of saturated batch-sorption and unsaturated transport-sorption approaches

K. Improved Spatial Discretization Techniques for 3-D Flow and Transport Models

Focus Area: Unsaturated Zone
Contact: Karsten Pruess, K_Pruess@lbl.gov, (510) 486-6732
Collaboration: LBNL

Statement of Problem

Numerical modeling has played a key role in understanding the flow and transport processes affecting fluid dynamics and radionuclide migration in the Yucca Mountain unsaturated zone (UZ) system. The accuracy of numerical simulations is critically dependent on spatial discretization (or gridding). Inappropriately designed numerical grids may introduce anything from mild inaccuracies to gross errors into the problem. Figures K-1–4 show gridding situations that may be typically encountered in modeling Yucca Mountain, for which current modeling techniques may produce potentially large and poorly quantifiable errors. This limits the reliability and credibility of model predictions.

Impact/Importance to the Yucca Mountain Project

Total system performance assessment (TSPA) relies heavily on flow and transport models for assessing the potential repository in the unsaturated zone (UZ). Numerical modeling has been a key tool for evaluating the effects of hydrogeologic, thermal, and geochemical conditions on various aspects of the overall waste disposal system. Whereas laboratory and field experiments are limited in both space and time, numerical modeling provides a means for studying large temporal and spatial scales relevant to understanding and quantifying physical processes associated with nuclear waste disposal in a geologic formation. Performance assessment models based on numerical simulation of water and gas flow, heat transfer, and tracer/radionuclide transport can include all known important physical and chemical mechanisms that affect the behavior of the potential repository and the host rock.

Flow and transport processes at Yucca Mountain occur in a structurally complex system of heterogeneous, layered, anisotropic, fractured volcanic rocks that are cut by numerous strike-slip and normal faults with varying amounts of offset. The major faults generally penetrate the complete UZ thickness, and to a certain extent control moisture flow and saturation distributions. Therefore, numerical gridding of Yucca Mountain has been a challenge and current modeling efforts are generally based on relatively coarse grid models because of the intensive computational requirements. A recent study (Wu et al., 2002) indicates that grid refinements may have significant impact on model results of percolation flux in the UZ.

Most performance assessment models are based on continuum modeling approaches and require control-volume type of grids (Pruess, 1991). Because of the complex geological features of Yucca Mountain, designing appropriate model grids has been an extremely difficult task. In general, irregular and unstructured grids have to be used, which makes it very difficult to ascertain the accuracy of such models. The work proposed here will develop rigorous methods for treating irregular geometries to permit a systematic evaluation and reduction of gridding errors, and thereby enhance the credibility of repository performance assessment.

Objective

A fundamental limitation of current space discretization techniques is that fluxes across grid block boundaries (interfaces) are calculated based on information from just two adjacent grid blocks. The objective of the proposed work is to introduce novel and more powerful geometric entities, specifically, "multi-block connections," that will permit a systematic evaluation and reduction of gridding errors. The new gridding approach will be developed and implemented into the TOUGH2 family of codes. In addition, the new gridding scheme will be used to design 3-D numerical grids for both continuum models and streamline-based models. The new gridding schemes are expected to significantly improve 3-D UZ model grids, for more efficient, accurate, and defensible modeling of large-scale flow and transport at Yucca Mountain.

Workscope

The work is subdivided into three tasks.

1. Define new geometry data types in TOUGH2. Assemble and code expressions for interface fluxes from multiple grid blocks, including all vectorial components of gradients, and appropriately interpolated mobilities and mass fractions.

2. Apply the new gridding method to unsaturated flow and transport problems that involve sloping layers, fault offsets, pinchouts, and local grid refinement.

3. Apply to full-scale 3-D models of Yucca Mountain for comparative study.

Schedule

Year 1: Formulate multi-node expressions for interface fluxes; code in TOUGH2; debug and test.

Year 2: Apply to 2-D cross sectional and 3-D models of Yucca Mountain.

Products

1. Improved formalism for treating complicated geometry of heterogeneous formations.

2. More accurate flow and transport models for Yucca Mountain.

3. Enhanced version of TOUGH2.

4. Laboratory reports and journal articles on space discretization effects for flow and transport models of Yucca Mountain.

5. Annual progress report to DOE

Level of Effort

1.5 FTE for two years.

References

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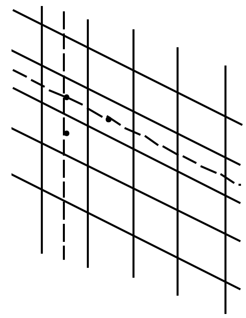

Figure K-1. For flow systems with sloping layers, lines connecting nodal points will not be perpendicular to interfaces

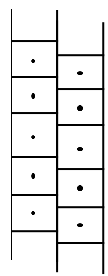

Figure K-2. At fault offsets, interfaces may involve more than two grid blocks

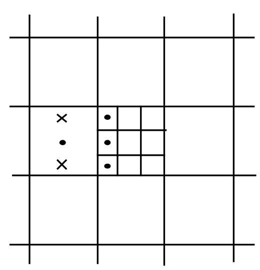

Figure K-3. Local grid refinement leads to non-orthogonal interfaces

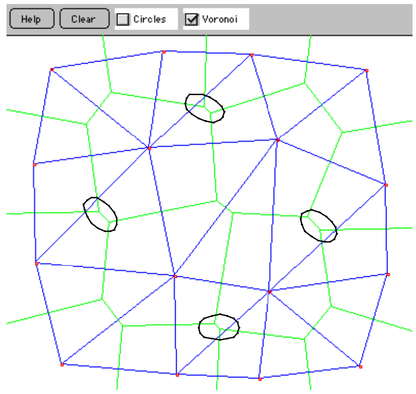

Figure K-4. General Voronoi grids may involve many interfaces that are “seen” under a small angle from nodal points, and are prone to large and poorly quantified discretization errors

L. Laboratory and Modeling Investigation into Reactive-Transport Parameters and Processes in the Unsaturated Zone

Focus Area: Unsaturated Zone and Near Field
Contact: Eric Sonnenthal, ELSonnenthal@lbl.gov, (510) 486-5866
Collaboration: LBNL

Statement of Problem

Reactive transport processes in the unsaturated zone (UZ) (including the near field) govern the chemical environment around drifts and must be evaluated in order to assess waste package corrosion rates and permanent effects of mineral alteration on flow and transport. Secondary minerals such as zeolites and clays modify the pH of water that could seep into drifts and contact waste packages. The reaction rate parameters and even the identity of these secondary mineral phases are poorly known for the conditions in the repository host rock at elevated temperaures and changes in partial pressures of CO_2. Reactive surface areas and the distribution of mineral precipitation in rough fractures are also very poorly constrained. The minerals coating the fractures and in contact with percolating waters are different from those making up the matrix of the tuff, for which previous experiments have been performed. No unsaturated water-interaction experiments have ever been done using natural fracture surfaces having the typical coatings of calcite, opal, fluorite, Mn-oxides, and stellerite observed in the devitrified welded host rocks of the potential repository. In addition, introduced materials, such as cementitious grout, will affect the sealing of fractures and the chemistry of water seeping into drifts. Therefore, the purpose of this work is to constrain mineral-water reaction rates and processes in individual mineral phases and in natural fractures of unsaturated tuff using both well-controlled laboratory experiments and reactive transport modeling.

Impact/Importance to the Yucca Mountain Project

The proposed work will have a direct impact on the assessment of uncertainty for the Yucca Mountain Project because it will provide a much stronger scientific basis for calculations of water and gas chemistry that may contact waste packages and affect corrosion rates. In particular, the results will include a much better constrained set of reactive surface areas, rate law formulations, and other chemical parameters for modeling water-rock interaction and boiling/evaporation processes in the near field and UZ. Results from the proposed experiments will form the basis for improved algorithms describing the kinetics of mineral dissolution and precipitation, and will result in greatly increased confidence in thermal-hydrological-chemical (THC) model predictions. This will greatly reduce uncertainty in the drift-scale and mountain-scale THC models that are used as inputs to engineered barrier system performance and UZ performance assessment. In addition to the natural system geochemical behavior, the added effects of water-rock interaction with cementitious grout in the emplacement drifts will allow for a better assessment of uncertainties in reactions and radionuclide transport in the UZ.

Quantitative modeling of the laboratory experiments would greatly benefit from extensions of the reactive transport modeling tools currently used for the Yucca Mountain Project. Therefore, a proposal to extend the TOUGHREACT code (Xu and Pruess 2001) to solve inverse problems and model high ionic strength fluids will enable bounding the reaction rate parameters from the experiments more easily and providing uncertainty ranges in predictions of water chemistry and permeability changes. The ability to capture geochemical preocesses in high ionic strength fluids will allow for a more complete transition from models used in the UZ to those used in the in-drift environment.

Objective

The overall objective of these combined laboratory and modeling studies is to quantify the reaction rate parameters and processes required to assess the water and gas chemistry which will in turn affect waste package corrosion rates.

The major scientific objective of the natural fracture experiments is to determine the relationship between reaction rates and liquid saturation and fluxes for mineral dissolution and precipitation processes. The sample will be a natural fracture, one side of which will be replaced by an inert transparent replica. This permits observation of the flow and, in particular, measurement of the areal coverage (the fraction of the fracture surface wetted by flowing water). Essentially, water will flow through the fracture at steady state, and flow rate, areal coverage, and influent and effluent analysis will be recorded. In addition to the effects of natural fracture mineralogy, the interaction of cementitious grout with mineral precipitation will be evaluated.

A comprehensive model for coupled reactive transport processes requires information at a variety of scales. In addition to the centimeter to decimeter scale of a fracture, basic information on the rates of reaction of individual natural minerals from fracture coatings are necessary. Therefore, we propose to determine non-linear mineral dissolution and precipitation kinetics far from and close to equilibrium, to predict accurately mineral reactions and their saturation under conditions similar to that expected in the near field. A related objective of this work is to incorporate a Pitzer-type model into the reactive transport code TOUGHREACT so that these reactive-transport processes can be investigated in the high-ionic-strength chemical regime. This regime could be be characteristic of the near-field environment where strong evaporation processes and interactions with cementitious grout will take place.

Workscope

Laboratory and modeling investigations will be integrated. Modeling simulations will be used to guide experimental conditions and for pre-test predictions and post-test analyses. Inverse techniques will be applied to estimate reactive surface areas (and other parameters) and to uncertainty analysis.

1. Laboratory investigation of mineral precipitation and dissolution in natural fractures

   Natural fracture surfaces are exposed when blocks separate or fall during mining. Several samples, about 0.4 x 0.4 m square, will be obtained. Samples will be obtained with both foot and hanging wall surfaces mated. For experiments, the natural footwall surface will be mated to a transparent replica of the hanging wall (see Figure L-1), prepared using the molding and casting techniques used by Su et al. (1999), or, preferably, a process of laser scanning and "rapid prototyping"*. This is a novel process in which a digital file controls the deposition of resin (or other material) to form solid objects. (The substrate could also be nontransparent but porous, to simulate imbibition). Resolution of this method is reported to be 20 microns. Finally, a second laser scan of the surface after the experiment can detect localized dissolution or precipitation (if greater than the resolution of this method, possibly 100 microns).

   If necessary to prevent the replica from participating in rock-water reactions, it can be coated with transparent teflon film (DuPont FEP), although this is a nonwettable surface. By adjusting the flow rate and the angle at which the assembled fractures are mounted, it should be possible to produce either steady or cyclically varying flow regimes with varying areal coverage ranging from 10% to 100%. Several replicas formed by rapid prototyping would be identical, which would allow a simple relationship between flux, angle, and areal coverage, a key variable to be investigated in these experiments and in simulations. (The glass, resin, or teflon surfaces of the hanging wall will be wettable to nonwettable by water, and this will affect the flow regime in the experiment. However, it is not expected to prevent the areal coverage from being controlled over a wide range.) Influent water will be pre-equilibrated either with the fracture minerals in a column or with cementitious grout. Flow rates and angles will be adjusted to cover a range of areal coverage, from, for example, 10–100%. Experiments will be run to hydraulic and chemical steady state. Influent and effluent water will be analyzed for major and minor chemistry and strontium isotopic ratios. Use of sensors eliminates the requirement to take samples, which can disturb the system.

* "Rapid prototyping" (RP) refers to the fabrication of a physical, three-dimensional part of arbitrary shape directly from 3D computer-aided design (CAD) data. Laser scanning creates the Unlike CNC machine tools, which are subtractive in nature, RP technology is an additive process that can generate free-from fabricated parts using powdered metals, polymers, paper, and other materials. Layer by layer, RP machines fabricate 3-dimensional objects based on this horizontal cross sections taken from a computer model.

2. Mineral Dissolution Rate Experiment

In addition to experiments that will quantify the interaction of water with a complex mineral assemblage on fracture surfaces, it is proposed to investigate the dissolution rate of natural Yucca Mountain minerals individually. This will allow for the fracture experiments to be interpreted in terms of the roles of the individual minerals in modifying the water chemistry. Our proposal is to measure dissolution rates with an alternative approach, using simple electrochemical cells of the type:

$$-Hg/HgO,\ Me^{z+}O_{z/2}/Hg^{2+},Me^{z+},OH^{-}/HgO/Hg+$$

where $Me^{z+}O_{z/2}$ represents the oxide component of any mineral that reacts with water to generate or consume OH^{-}. Details of the cell design and function are given in Berecz and Szita (1970; see Figure L-2). During dissolution of a mineral, an electrical potential is generated across the cell, which is a function of the degree of disequilibrium, and is directly related to ΔG_r, the Gibbs free energy of the dissolution reaction. This potential declines to zero as equilibrium (saturation) is attained. Monitoring and recording of the potential is easy, allowing acquisition of a continuous record rather than discrete data points. Initial conditions and temperatures to 100 ^{o}C can be specified. Incorporation of an oxide electrode system to continuously monitor pH might be feasible. Data acquisition should be far greater, more rapid, and more precise than previous methods using flow-through cells (e.g., see Lasaga and Luttge 2001). Berecz and Szita demonstrated the use of their cell in measuring the dissolution of gibbsite. Modifications of the cell design could be used where highly viscous solutions are involved, as in reactions in the presence of high ionic strength salt solutions simulating processes in crevices of waste containers.

Specific Laboratory Tasks:

1. Water-Rock Interaction in Single Natural Fractures (see description above and Figure L-1)

   1.1 Obtain natural fractures based on mineral assemblages on fracture surface, in particular those having Mg-enriched calcite, opal, fluorite, and stellerite.

   1.2 Characterize the mineral proportions, compositions, and geometric surface areas (prior to and after the experiment).

   1.3 Run a series of experiments covering a wide range of liquid fluxes, water saturations and temperatures and different initial water compositions (including various natural isotopic systems and water equilibrated with cementitious grout).

   1.4 Use inverse methods to determine reactive surface areas for mineral precipitation and dissolution.

2. Mineral Reaction-Rate Experiments

   2.1 Design and fabricate cell.

   2.2 Purchase water bath, high impedance voltmeter data logger (to record cell emf, pH, and temperature).

   2.3 Prepare sample materials (tentatively: kaolinite, smectite, albite, plagioclase feldspar, hematite and stellerite, or other zeolites from fractures in repository host rocks).

   2.4 Collect data.

2.5 Develop a cell model simulator (to aid in data analysis and interpretation).

2.6 Interpret data and construct a suitable kinetic algorithm for incorporation into TOUGHREACT.

Specific Modeling Tasks:

1. Adapt inverse techniques to reactive transport code TOUGHREACT.
2. Incorporate *Pitzer module* (already developed by Zhang and Zheng, unpublished) into TOUGHREACT.
3. Perform pre-test reactive transport modeling and post-test inverse modeling to derive parameters and uncertainties.
4. Model existing Yucca Mountain alteration using new rate law data.

Schedule

Year 1:

A. Set up and run ambient single natural fracture temperature laboratory experiments (including cementitious grout).

B. Set-up and run mineral reaction rate experiments.

C. Incorporate *Pitzer module* into TOUGHREACT.

D. Incorporate inverse modeling capabilities into TOUGHREACT.

E. Perform pre-test predictive modeling of lab experiments.

F. Write and submit papers on low-temperature results (experiments and modeling).

Year 2:

G. Complete high-temperature single natural fracture reactive-transport experiments.

H. Complete mineral reaction-rate experiments.

I. Perform post-test forward modeling of experiments.

J. Perform post-test inverse modeling of experiments.

K. Perform long-term modeling of Yucca Mountain using new rate law data.

L. Write and submit papers on high-temperature results (experiments and modeling).

Products

Products include publication of papers documenting processes and parameters for unsaturated reactive transport in natural fractures in high- and low-ionic-strength fluids. An algorithm will be developed describing mineral nonlinear dissolution/precipitation kinetics for incorporation in reactive chemical transport codes. This will also include specific reaction rate parameters specific for Yucca Mountain. The effects on the alteration of the near-field environment and subsequent effects on water chemistry, potentially affecting waste package corrosion, will be assessed.

Level of Effort

Laboratory Studies: 1.5 FTE first year, 1 FTE second year

Equipment/Analytical Costs:

Fracture Flow Experiments – $25,000.

Mineral Reaction-Rate Experiments – $6,000.

Modeling Studies: 2.0 FTE first year, 2.0 FTE second year

References

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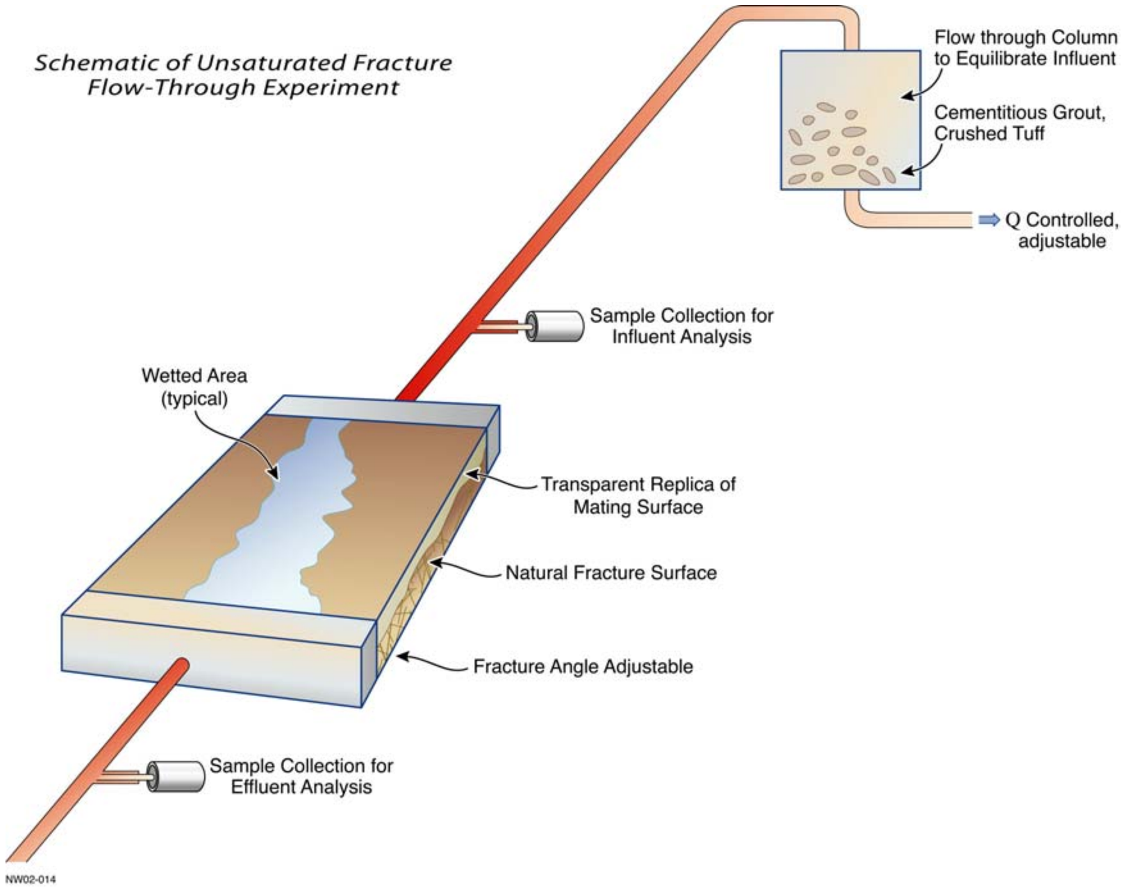

Figure L-1. Schematic diagram of proposed fracture flow-through reactive transport experiment.

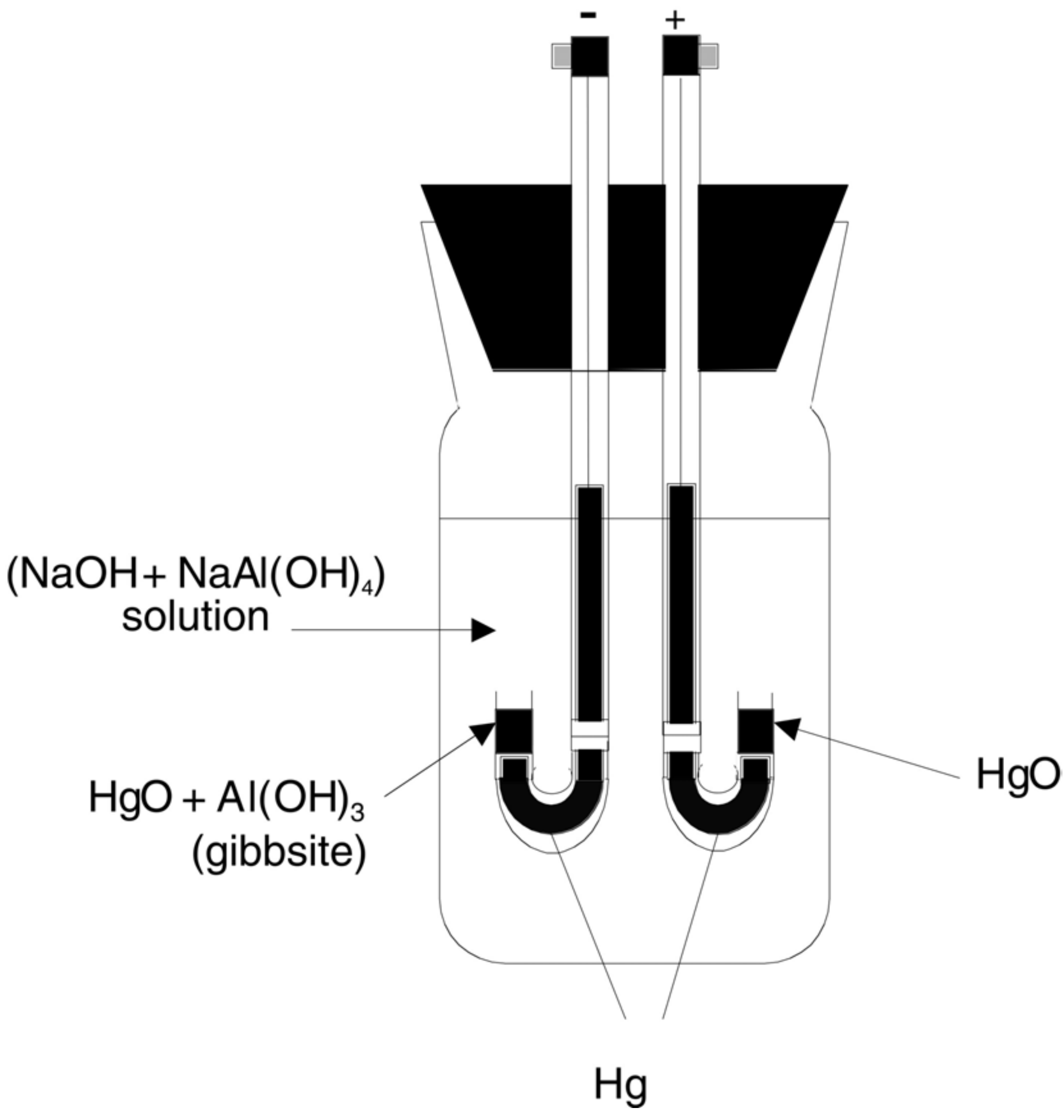

Figure L-2. Schematic design of an electrochemical cell for measurement of mineral hydrolytic dissolution kinetics (after Berecz and Szita, 1970).

M. Thermal-Chemical and Thermal-Mechanical Effects on Fracture and Matrix Properties

Focus Area: Near Field
Contact: Timothy J. Kneafsey, TJKneafsey@lbl.gov, (510) 486-4414
Collaboration: LBNL

Statement of Problem

During the construction and operation of the proposed nuclear waste repository at Yucca Mountain, Nevada, several types of changes will take place in the rock properties near the repository drifts that will affect the long-term performance of the repository, including mining damage and changes caused by heating. First, mining the drifts will damage the nearby rock. Second, the emplacement of heat-generating nuclear waste will heat the rock, causing rock expansion and vapor and liquid flow.

Mining of underground drifts changes the stresses in the host rock, often inducing additional fracturing in the host rock near the drifts (damage zone). The extent of this damage zone may be on the order of a drift diameter into the host rock. In addition to mining-induced fracturing, dust from the mining activities will tend to fill fractures, particularly on the lower portions of the drifts. The increased fracturing and dust infilling will result in changes to the permeability that will affect seepage, flow, and transport near the drifts.

When a drift is heated, the properties of the fractures and matrix are expected to change. Heating will induce expansion of the rock, altering the stress field, fracture aperture, and permeability. Heating will also induce evaporation of the water from within the porous fractured rock, causing vapor migration in fractures and condensation upon meeting cooler rock. Condensed water above the heated drifts will flow downward, dissolving the local rock minerals. As it flows towards the heated drifts, the water will be evaporated, leaving the dissolved constituents behind. The continuous repetition of this cycle will result in reduced fracture apertures, fracture wall coating, and fracture plugging, which affect permeability and fracture-matrix interaction. Other effects of increased temperature include changes in water properties such as water surface tension and viscosity. These properties both decrease, affecting capillary pressure (which affects pressure gradients and capillary condensation) and water flow, particularly imbibition into the rock matrix.

Proper incorporation of the permeability changes caused by all of these effects into performance assessments of Yucca Mountain is necessary to reduce uncertainties and improve predictions. We propose experiments in single fractures, foot-scale blocks containing a fracture network, a meter-scale block containing a fracture network, and in the field in addition to using numerical modeling to investigate these problems.

Impact/Importance to the Yucca Mountain Project

Knowledge of thermal-mechanical and thermal-chemical effects on permeability changes in the near-drift zone is important for improved predictions concerning the potential nuclear waste disposal site at Yucca Mountain. Because of the stress condition at Yucca Mountain and the changes that may occur resulting from heating, determination of stress-permeability relations for Yucca Mountain tuffs will increase the accuracy of predictions of flow around drifts. A better understanding of mineral precipitation in fractures will also provide for better predictions, because these permeability alterations will remain when the repository cools. The added understanding will allow for a more realistic evaluation of drip shield need, potentially providing significant cost savings. More accurate flow and seepage modeling will allow for evaluating the reduction in risk of radionuclide release provided by the natural system. Previous experimental work performed to understand fracture plugging in unsaturated fractures caused by mineral precipitation showed fracture plugging in a very short time. This work was limited to a homogeneous planar aperture (Dobson et al., in press). In this earlier work, only a thin band of precipitate was needed to strongly reduce permeability. Examples of these thin bands, or bridging structures were observed throughout the superheated zone (Figure M-1). Fracture plugging in a heterogeneous unsaturated fracture is hypothesized to occur in the thinner aperture regions first, because capillary forces will strongly affect the flow location. Later flows will then be confined to larger apertures where flow will be faster, influencing seepage. The possible extent of chemical sealing is not known because of conflicting results of laboratory and modeling studies.

Chemical sealing could have a huge impact on the performance of the repository and could dominate the response of the system; therefore, this issue requires resolution.

Objective

The primary objective of this work is to understand the effects of property changes caused by thermal-mechanical and thermal-chemical changes on flow, transport, the shadow zone, and seepage. Specific goals include:

1. Enhancing understanding of the permeability changes in single fractures and a fracture network caused by varying stress. The following will be determined: (a) the ranges of residual permeability (minimum limit of permeability at high stress), (b) the ranges of induced permeability changes under varying normal stress, (c) the impact of initial permeability on the stress versus permeability function, and (d) the impact of fracture shear on the stress versus permeability function.

2. Enhancing understanding of the genesis of fracture plugging caused by mineral precipitation in a fracture containing known heterogeneities (created in natural rock), and in a natural fracture network. We will observe (a) the changes in permeability over space and time and how the mineral precipitation occurs in relation to an imposed aperture distribution and temperature gradient, and (b) how the spatial and temporal formation of mineral precipitate in a well-characterized natural fracture network affects permeability over time.

3. Enhancing understanding of the changes in flow and imbibition caused by thermally induced surface tension and viscosity changes. We will measure the bulk effects of water property changes caused by temperature on imbibition, so they may be included in simulations of repository performance. These changes in the physical properties of water will affect the characteristic curves used in numerical modeling at Yucca Mountain.

4. Defining the extent of the damaged zone. Geophysical techniques will be applied to quantify the effect of mining on the host rock.

Workscope

1. Thermal-Mechanical Effects on Fracture Flow

   To determine the stress versus permeability relationship for Yucca Mountain tuffs, laboratory experiments will be performed to evaluate the normal stress versus permeability relationship for a number of important fracture types under different shear offsets. Permeability will be measured across a range of normal stresses for a fracture. A small shear displacement will be induced and a new normal stress versus permeability curve will be determined for the same fracture. In this way, the impact of shear on the resulting stress-permeability function will be evaluated. An example of expected results is shown in Figure M-2. Measurement of a stress-permeability relationship in a fracture network will be performed by applying a normal stress to foot-sized test blocks containing intersecting fractures and measuring permeability. The results of the stress-permeability functions determined here will be used in future modeling to provide better predictions of repository performance.

2. Thermal-Chemical Effects on Fracture and Matrix Flow

   Three experiments are proposed to evaluate thermal-chemical effects on fracture permeability. In the first test, water containing dissolved mineral constituents will be introduced into a foot-scale fracture containing a known (created) aperture distribution in Yucca Mountain tuff and a known temperature distribution. The aperture distribution will be pre-set to test the hypothesis that sealing occurs initially in the smaller apertures for low flow rates, confining later flows to larger apertures (and causing faster flows). The permeability of the fracture and the accumulating solid precipitate volume will be monitored over time. This information will be used to evaluate the structure of any flow blockage in the fracture. If applicable, linear or computed tomography (CT) x-ray scanning will be used to help evaluate the effect of mineral precipitate on permeability from the fracture to the matrix. To further validate the resealing process of the fracture, seismic imaging will be used. Previous application of seismic imaging on a field scale has shown how strongly seismic-wave propagation is affected by changes in fracture aperture, because the aperture and fracture content control the fracture stiffness and hence the mechanical properties that influence seismic wave propagation. Seismic experiments will be conducted to determine the properties of the transmitted and reflected wave fields as a function of mineral precipitation and changes in aperture.

The second test will use a natural fracture network within a foot-scale block of tuff. Again, water containing dissolved mineral constituents will be introduced into a well-characterized block maintained with a temperature gradient. Intermittent monitoring of the gas-phase permeability and volume of precipitated solids will be used to understand the changes to the permeability structure. Seismic imaging will be used to determine how the results of imaging a single fracture compare to those of a fracture system. Doping the influent water with an x-ray attenuating solute may be used so that the location where precipitate occurs can be observed spatially and temporally using x-ray scanning.

The third test will be performed in the meter-scale block. We will characterize the block and induce flow at various rates under isothermal and moderately non-isothermal conditions. We will monitor the temperature distribution and changes in spatial and temporal flow occurrences with flow rate and applied thermal gradient. The understanding gained in these tests will be used to revise conceptual models for fracture plugging that can be extended using numerical modeling and used for better predictions of repository performance. Flow variation in the foot-scale blocks with thermal-hydrological-mechanical and thermal-hydrological-chemical changes will be compared with flow through a meter-scale block, used to identify natural flow pathway variations.

3. Thermally Induced Changes in Water Properties

Changes in water properties at increased temperatures will affect water's ability to flow. Imbibition into the matrix is expected to increase due to the increased ratio of interfacial tension and viscosity. This phenomenon will be investigated by performing a limited number of imbibition experiments. The results will be incorporated into numerical models of flow and transport near the repository. An extensive review of the literature on this subject will also be completed prior to the initiation of this experimental work.

4. Field Measurement of the Damage Zone

Large-scale seismic imaging has been successfully conducted at Yucca Mountain to determine the fracture density throughout the repository horizon (Gritto et al. 2002). Seismic velocity estimates from tomographic studies were converted (based on composite medium theory) to determine the fracture density throughout the repository, which correlated well with fracture mapping along the tunnel walls (Figure M-3). A similar approach on a smaller scale and with higher resolution can be applied to study the damaged zone around drifts at Yucca Mountain. Seismic sources and receivers can be deployed in existing and new boreholes drilled from the tunnel walls into the damaged zone. At other locations (i.e., Nevada Test Site) the damaged zone has been found to extend about one tunnel diameter out into the host rock. We plan to use high frequency seismic borehole sources (1-10 kHz) producing wavelengths in the tens of centimeters to meter range, such that the resolution is expected to be less than one meter. Tomographic velocity estimates will be converted to fracture density, which is a direct indication of the degree of damage. Furthermore, fracture orientation will be estimated to determine the degree of fracture anisotropy. The results will provide a set of necessary parameters that will be incorporated into numerical models, which evaluate the effect of tunnel damage on seepage (see Task 5).

5. Numerical Evaluation of the Effects of Property Changes caused by Thermal-Chemical and Thermal-Mechanical Effects

   A study will be performed to evaluate the impact of near-drift property changes on seepage under thermal and ambient conditions. This study will consist of (a) reviewing existing data on property changes due to mining at Yucca Mountain and a comparison of the effects of different mining technologies, (b) reviewing data from other sites, (c) evaluation of the combined effects of mining and thermal-chemical and thermal-mechanical changes, resulting in property estimates after the thermal period, and (d) numerical studies on the effects of the property changes on seepage, transport, and the shadow zone. The numerical studies will be based on property ranges determined in Tasks 1–4. The modeling will be three-dimensional and contain stochastic heterogeneous property (permeability and porosity) distributions.

Schedule

Many of the tasks described in the work scope above can be completed in parallel. The following table describes the anticipated schedule of completion, estimated level of effort, and need for equipment.

Task	Anticipated Completion	Estimated Level of Effort	Equipment Needed
1	Year 1 and 2	1 FTE	Yes
2	Year 1 and 2	1.5 FTE	Yes
3	Year 1	0.5 FTE	No
4	Year 1 and 2	0.5 FTE	Yes
5	Year 2 and 3	0.5 and 2 FTE	No

Products

One report will be submitted to the Yucca Mountain Project, and at least one journal article will be submitted for each task above. Additionally, a status report will be submitted annually to the Yucca Mountain Project.

References

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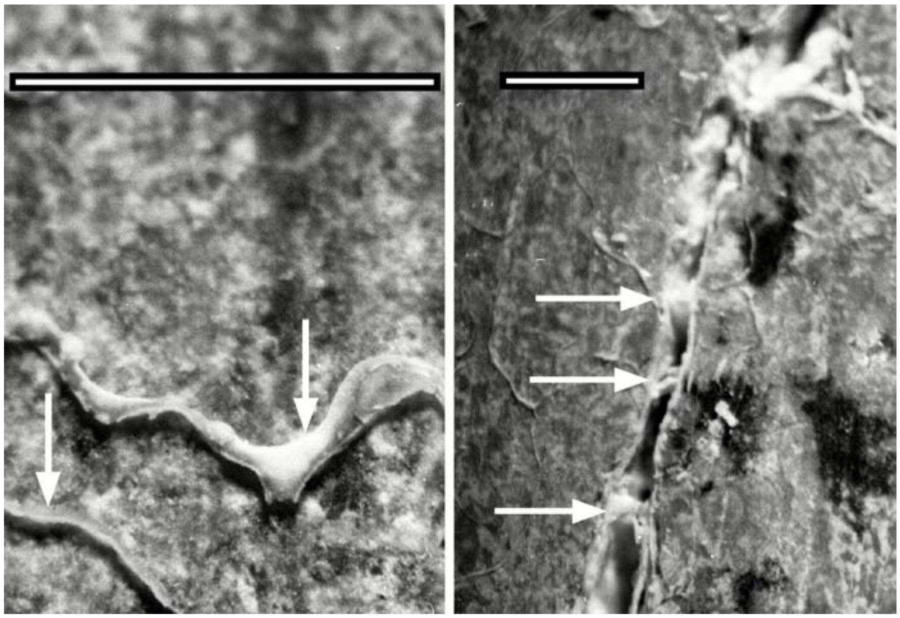


Figure M-1. Bridging structures in an opened planar fracture (left) and in a crosscutting fracture (right). Scale bars are 1 mm.

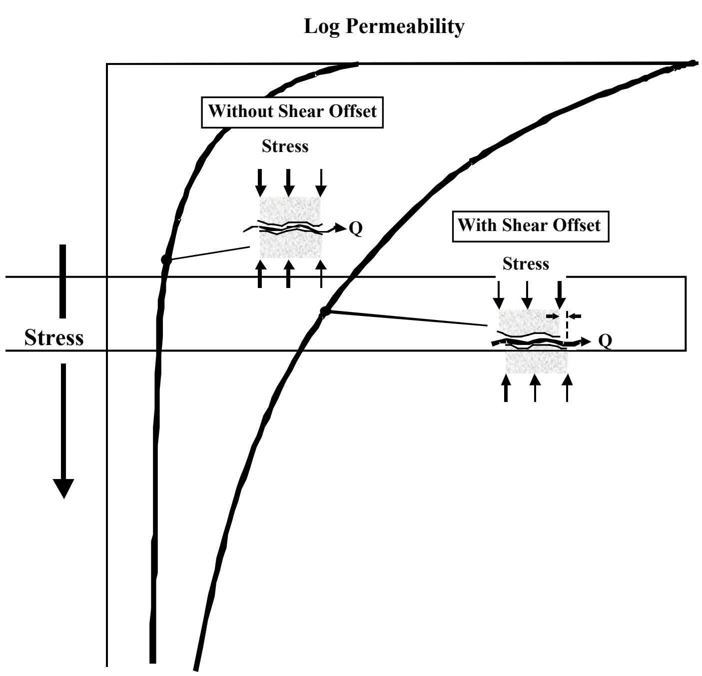


Figure M-2. Stress versus permeability curve.

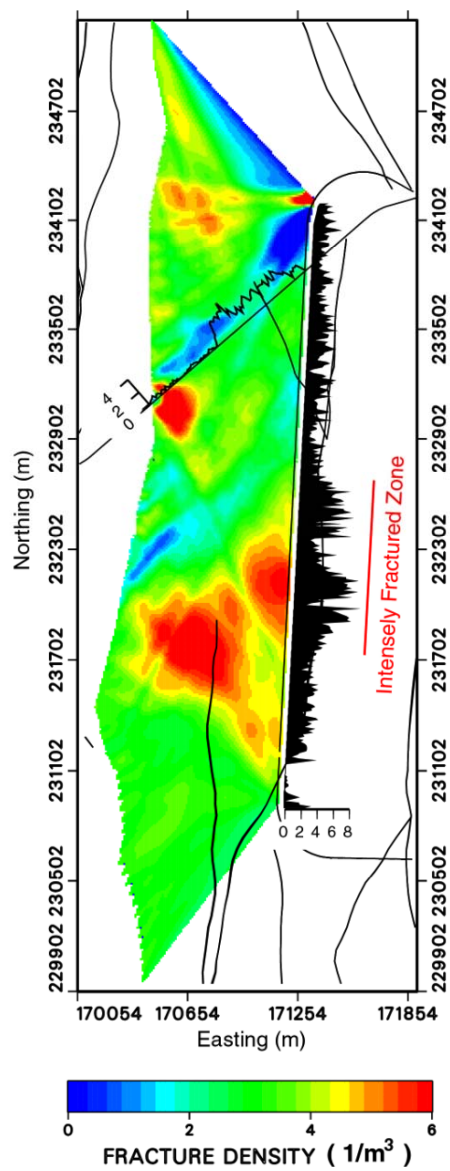


Figure M-3. Fracture density estimated using geophysical methods near the main drift of the ESF and measured fracture density at the drift wall.

N. Multiscale Thermomechanical Effects of Magma Intrusion on Drifts and the Unsaturated Zone

Focus Area: Unsaturated Zone
Contact: C.M. Oldenburg, CMOldenburg@lbl.gov, (510) 486-7419
Collaboration: LBNL

Statement of Problem

Although controversy exists concerning the probability of magma intrusion into the area of the potential repository at Yucca Mountain (Smith et al., 2002), there is little doubt that the effects of such an event would be profound. In particular, magma may either vesiculate and erupt explosively into the drifts, or it may enter the drifts as a viscous lava flow and slowly solidify. Depending on which scenario occurs, the drifts and surrounding unsaturated zone (UZ) will be forever changed after filling with tephra or molten rock with the potential for mechanical stoping and melting of wallrock. In addition, regardless of the mode of discharge, magma intrusion in general will supply large amounts of heat to the formation altering the ambient thermal, stress, and moisture regimes on both the drift and mountain scales. In order to assess the impacts of magma intrusion on waste isolation and transport, it is necessary to understand the processes associated with magma intrusion on the wallrock, drift, and mountain scales.

Impact/Importance to the Yucca Mountain Project

Volcanoes and hydrothermal manifestations of magmatic heat are dramatic events that capture wide public attention. As the only recognized potential contributor to radionuclide dosage in the first 10,000 years, it is essential to understand the processes involved in magmatic intrusion and the effects of magmatic intrusion on drifts. Prior work on probabilities of magma-drift intersections was complemented by consequence studies that most often rely on analytical approaches and scale analysis that involves conservative assumptions and end-member or worst-case scenarios. Our approach will involve detailed process simulation to model more realistic cases of magma-drift interaction and effects. Added realism usually leads to decreased consequences relative to worst-case scenarios. The research proposed here will inform the Project about the potential effects of magma-drift interaction on the wallrock, drift, and mountain scales. The results of this project are needed to assess the potential for radionuclide transport resulting from short-term and long-term effects of magma intrusion.

Objective

The objective of this research is to understand thermal, mechanical, and moisture effects associated with magma intrusion into drifts in the UZ at Yucca Mountain. The scientific issues to be addressed include heat transfer from the magma to the formation near the drift, geochemical effects of magma-wallrock interactions, normal, shear, and thermal stresses arising from magma flow on canisters and drift walls, potential for explosive events as opposed to viscous flow in the drift, moisture boiling and migration due to heating, and solidification and convection within the magma. The approach will build on years of past experience by the research team in the areas of volcanology and magma dynamics, geochemistry, igneous petrology, and rock mechanics. Because recorded cases of magma intruding into tunnels have not been found to use as analogues, the approaches consist of numerical simulation, geochemical and volcanological modeling, and igneous petrology.

Workscope

1. Establish the expected range of composition of the magma that may intrude at Yucca Mountain.

   This task will build upon the work already carried out by the project to estimate plausible compositions of future magmatic intrusions. The key properties of magma that determine its eruptive intensity and style are its composition in terms of silica and volatile (mainly water and carbon dioxide) content and degree of crystallization (Papale et al., 1999). Highly siliceous and water-rich magmas are the most explosive due to the rapid exsolution of water from the silica-rich viscous melt upon decompression resulting from the ascent of magma. Another important factor that can affect explosivity is the amount of groundwater that interacts with the intruding magma, a process that can result in phreatomagmatic eruptions. After reviewing the existing work and related literature on compositions and textures of volcanic rocks from cinder cones in the Yucca Mountain area, and considering potential variations that arise from the passage of magma through the basement rocks at Yucca Mountain, this work will define a likely range of compositions of future magma that may intrude into the drifts at Yucca Mountain. If needed, additional analytical work may be conducted to measure volatile contents of previously erupted magmas, for example using FTIR (Fourier transform infrared spectroscopy) methods on glass inclusions in phenocrysts.

2. Determine the style of magma discharge as a dike intersects a drift.

   Depending on the magma composition and supply rate, magma that intersects a drift may erupt violently into the drift, or enter the drift as a viscous lava flow (Figure N-1a and b). From the likely compositions defined in Task 1, the expected explosiveness of magma intruding into a drift will be assessed. In addition to magma composition, the ability of the dike to supply magma is a key issue. For example, the magma composition and drift pressure may result in explosive volcanic behavior. If the dike is narrow and the magma supply rate correspondingly limited, the eruption into the drift will not be sustained. On the other hand, a high magma supply rate from the dike could provide sufficient mass flow rates to supply significant eruptive activity through the drift. The approach used for these analyses will be a combination of scale analysis and numerical simulation. Based on magma composition, degree of vesiculation and crystallization, and temperature profiles estimated for the dike and drift, an estimate of magma viscosity can be made. From dike width and magma viscosity, magma supply rates can be estimated and simulated.

3. Assess magma-drift interaction under explosive and lava flow discharge modes.

   The goal of this task is to determine the nature of the interaction of magma and the drift. When the magma discharges through the drift, shear and thermal stresses associated with flowing magma may cause significant stoping and transport of fractured blocks plucked from the drift walls (Figure N-1c and d). When hot magma from the dike encounters cooler wall rocks, crystallization and geochemical reactions such as partial melting and assimilation of the stoped blocks will occur as the melt solidifies. Meanwhile the core of the lava flow in the drift may stay hot, analogous to lava tubes formed during surface or subsea lava flows by cooling and solidification of the outer surface of lava while the core remains molten and mobile. Using numerical simulation of the relevant flow equations, we will simulate the explosive and lava-flow modes of magma discharge through the drift with a focus on how far magma will travel in the drift and what effects it might have on the wallrocks. Geochemical modeling will be used to constrain potential interaction of the welded and nonwelded tuffs at Yucca Mountain with the intruded magma.

4. Assess the potential transport of waste by the intruded magma.

   Shear and thermal stresses arising from lava flow in the drift will tend to deform waste canisters and transport them and any spilled contents along with the lava. However, if solidification occurs quickly, the potential exists for the magma to entomb the waste canister before significant deformation and transport can occur. We will use numerical simulation to explore conditions under which the waste canister would be entombed by magma as opposed to sheared apart and transported by the magma. The essential question is whether flowing lava in the drift would tend to flush material from the drifts or tend to enclose and smother it without significant transport from the drifts.

5. Assess the effects of drifts on magma intrusion in terms of the scale of the mountain and scale of the drifts.

   The purpose of this task is to elucidate the degree to which the drifts affect the overall ascent of magma in the dike at the scale of Yucca Mountain (Figure N-2). A simple scale analysis that compares the volumetric flow rates of magma, as constrained by cooling processes in the dike, with magma flow rates in the drifts, will show how much the drifts can be expected to alter the overall magma transport in the dike. The vast difference in scale between the mountain and the drifts suggests that the drifts will play little role in overall magma transport should such an intrusive event occur.

6. Assess the post-intrusion hydrology.

   The intrusion of a dike is expected to be accompanied by significant changes in the stress state of the rock around the drift, with associated failures of fractured welded tuff. These changes in stress will arise from both thermal and mechanical changes associated with the intrusion of hot magma. Numerical simulations will model the coupled hydrothermal-mechanical effects of magma intrusion on the fractured and nonwelded tuffs at Yucca Mountain. These effects will alter the fracture systems and therefore affect the permeability. We will carry out coupled moisture migration and magma cooling simulations to assess post-intrusion moisture distributions and the corresponding potential transport of leaking waste.

Schedule

Year 1: Tasks 1 and 2.

Year 2: Tasks 3, 4, and 5.

Year 3: Task 6.

Product:

Annual progress reports. In addition:

Year 1: Report on magma compositions and discharge style.

Year 2: Report on magma-drift interaction, waste transport, and overall effects of drifts on magma transport. Journal article to be submitted on subject of magma-drift interaction.

Year 3: Report on post-intrusion effects. Journal article draft on post-intrusion effects.

Level of Effort:

Year 1: 1 FTE.

Year 2: 1.5 FTE.

Year 3: 1.5 FTE.

References

Papale, P., A. Neri, and G. Macedonio, 1999. The role of water content and magma composition on explosive eruption dynamics, Phys. & Chem. of the Earth Part A–Solid Earth and Geodesy, 24(11-12), 969–975.

Smith, E.I., D.L. Keenan, and T. Plank, 2002. Episodic volcanism and hot mantle: Implications for volcanic hazard studies at the proposed nuclear waste repository at Yucca Mountain, Nevada, GSA Today, 12(4), 4–10.

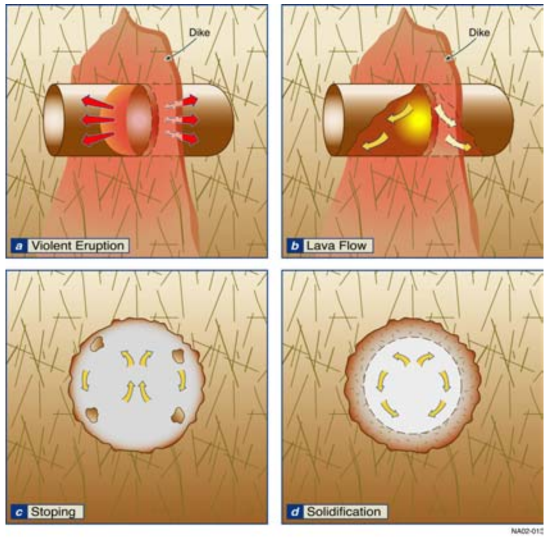


Figure N-1. Schematic of (a) explosive and (b) lava-flow scenarios for magma discharge through drifts, along with cross-section schematics of magma in drift causing (c) stoping and (d) solidification against the drift walls.

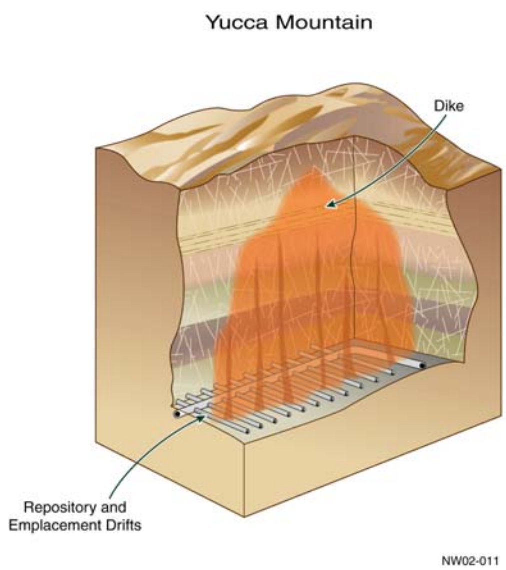


Figure N-2. Mountain-scale schematic of dike intersecting drifts

O. Building Confidence in Nuclear Waste Isolation through Natural Analogues

Focus Area: Natural Analogues
Contact: A. Simmons, AMSimmons@lbl.gov, (510) 486-7106
Collaboration: LBNL with USGS, LANL, LLNL, BSC

Statement of Problem

Predicting with confidence the behavior of the in-drift environment and components of the natural and engineered barriers over long time periods and large spatial scales is not usually amenable to testing by laboratory and field experiments. Natural analogues offer the opportunity to observe processes over the long-term. Analogues can also be used to determine the range of applicability of models and to assure qualitatively that the appropriate processes and sub-processes are included. In these ways, natural analogues provide corroborating information that can be used by Yucca Mountain Project (YMP) process models. The Nuclear Regulatory Commission (NRC), in final rule 10CFR63.101(a)2 (66FR55732)], has stated that natural analogues are one means of demonstrating compliance as a supplement to complex predictive models that are supported by limited field data and observations.

Impact/Importance to Yucca Mountain Project

The proposed work will improve the mechanistic understanding of processes, validate conceptual models, and, in some cases, verify numerical models. With analogue information used to substantiate the approach and methodology deployed at Yucca Mountain, both the public and the scientific community can be more convinced that Yucca Mountain is a suitable site for a nuclear waste repository. It is therefore critical to support and emphasize the natural analogue studies as the Project moves forward from site characterization to license application and performance confirmation phases.

Objective

The primary objective of the proposed natural analogue studies is to build confidence in the ability of the Yucca Mountain engineered and natural barrier systems to isolate waste for long time periods and over large spatial scales. The natural and anthropogenic analogue studies proposed will increase confidence in the unsaturated zone (UZ) flow and transport models under ambient and repository conditions, considering the effect of the drift opening on flow, the effects of degraded man-made materials and the presence of microbes on transport. The Peña Blanca study is also intended to increase confidence in waste isolation within the waste form. Existing data for some analogue sites will be supplemented by collection of additional data from field investigations. The data will be used to test conceptual models and will provide input for numerical models of reactive transport and site-scale transport.

Workscope

The proposed natural analogue studies are described individually on the following pages. Each one is a discrete project with the following components:

- Assembly of existing information and data
- Initial conceptual model development and pre-test modeling
- Data collection through fieldwork and experimentation
- Data interpretation and analysis
- Predictive modeling and application to YMP

O.1. Peña Blanca

Statement of Problem

The Peña Blanca site affords a setting to test models of UZ flow and transport, SZ flow and transport, and waste form degradation as it influences the source term. Process models that support the YMP performance assessment model have not been tested using information from a similar field site that could provide insights into long-term conditions and processes. Although the Project has used supporting information from a number of natural analogue sites to corroborate such things as the rate of matrix diffusion, the role of colloids in transport, and the formation of secondary minerals in a waste form analogue, no analogue has been studied to test entire process models.

Impact/Importance to Yucca Mountain Project

Peña Blanca is the only analogue site thus far identified that possesses numerous similar attributes to Yucca Mountain in geology, hydrologic setting, climate, mineralogy, and size of uranium deposit. Of all the analogue sites explored in the literature or in person, Peña Blanca comes the closest to being a total system analogue. It offers the additional advantage that previous studies have characterized the site and the surrounding region in considerable detail, providing important supporting information for conceptual and numerical models.

Objective

The primary objective is to develop a conceptual three-dimensional model of transport of uranium and radiogenic daughter products at the Nopal I uranium mine in Peña Blanca, Mexico. Results of these tests are intended to provide added confidence in models of UZ and SZ flow and transport and waste form secondary-mineral sequestration by investigating uranium transport away from a uranium deposit in unsaturated welded ash flow tuff. Some of the processes that will be addressed are advective transport in fractures, sorption onto fracture coatings, retardation in secondary minerals, and plume dispersion.

Workscope

1. Perform U-series analyses of core and cuttings

   Results of analyses of hand samples previously collected at the site were reported in *Natural Analogues for the Unsaturated Zone,* ANL-NBS-HS-000007, Rev 00 (CRWMS M&O 2000a) and in the *Natural Analogue Synthesis Report,* TDR-NBS-GS-000027, Rev 00, ICN 02 (BSC 2002). The immediate focus of new work will be on U-series analyses of core and cuttings collected from three deep boreholes, modeling and interpretation of U-series results, collecting and analyzing water samples from the boreholes (see Figure O-1), and obtaining additional water samples from a water collection system in the Nopal I mine adit, Level 00 at Peña Blanca.

2. Collect additional water samples

   Additional water samples will be collected from available active local wells, and from the water collection system in the adit-access tunnel at Level 00 of Nopal I. The water samples will be collected at three-month intervals four times per year. The waters will be analyzed for major ions and composition of strontium isotopes, stable isotopes, uranium-series isotopes, and colloid content.

3. Extend conceptual model of uranium transport to 3-D model

   The conceptual model of uranium transport (CRWMS M&O 2000, BSC 2002) will be extended to the third dimension, incorporating information gained from study of core and cuttings pertaining to matrix diffusion and secondary mineral sequestration, hydrologic data (Green et al. 1995), and chemical, isotopic, and colloidal analyses resulting from this study. The data will be used as input parameters for a UZ flow and transport model that employs the same tools and techniques as used for the YMP UZ models. Evolution of the model may necessitate drilling several additional wells to further constrain the model. The Nopal I adit would be an ideal location for testing drift shadow zone behavior (see Proposal H); additional boreholes to accommodate workscope for this purpose could easily be drilled and instrumented, but would be in addition to those proposed below.

4. Perform petrographic optical microscopy analysis

   Petrographic analysis of thin sections made from Peña Blanca core samples will be performed by optical microscopy. Scanning electron microscopy may be used to analyze selected fracture-filling materials and other secondary minerals in and around the ore body. Analysis of isotopic composition (uranium-series and technetium) of solid and water samples will be performed using Thermal Ionization Mass Spectrometry (TIMS).

Tasks

Task 1: Drilling, geophysical logging, and initial core and water sample collection

Task 2: Chemical and isotopic analysis of water samples

Task 3: Petrographic analyses of core samples

Task 4: Extension and refinement of conceptual model

Task 5: Numerical model of UZ flow and transport

Task 6: Waste form degradation model

Task 7: Numerical model of SZ flow and transport

Task 8: Prediction and application to YMP

Task 9: Preparation of final reports

Product

An annual progress report will be submitted to DOE. Results of the work will be published in journal articles. The *Natural Analogue Synthesis Report* will also be revised to reflect the results of this work.

Level of Effort

The schedule and anticipated level of effort for each task are shown in the following table:

Task	Year 1	Year 2	Year 3
1	3 FTE	¼ FTE for additional water samples in each of FY04 and FY05. Additional cored and completed drillholes are ~$50k each; with cuttings only, the cost is ~$30k.	¼ FTE for additional water samples in each of FY04 and FY05. Additional cored and completed drillholes are ~$50k each; with cuttings only, the cost is ~$30k.
2	1 FTE	2 FTE	½ FTE
3	1 FTE	1 FTE	—
4	½ FTE	½ FTE	—
5	—	1.5 FTE	½ FTE
6	—	1 FTE	½ FTE
7	—	1 FTE	½ FTE
8	—	—	3/4 FTE
9	—	—	1.5 FTE

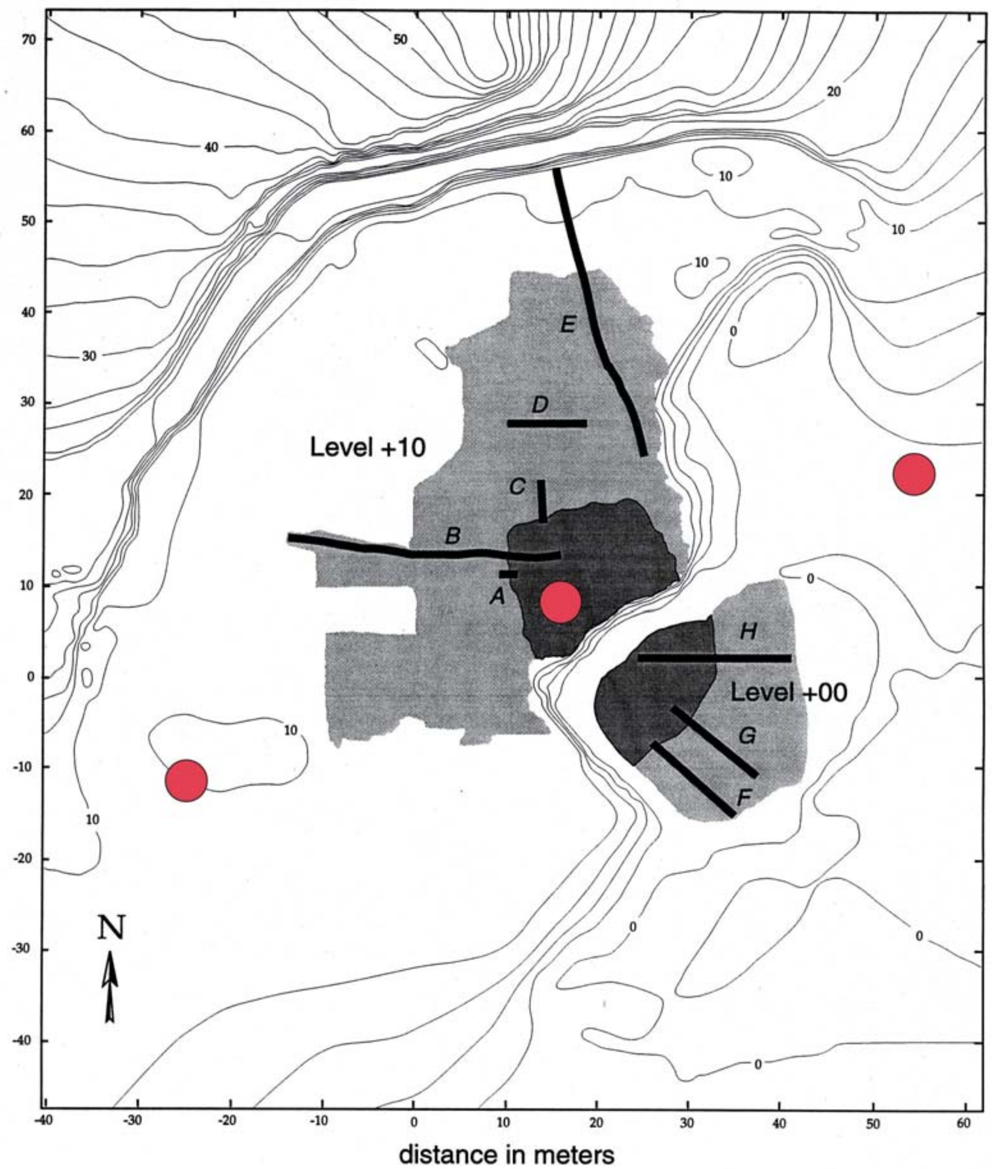


Figure O-1. Map of Peña Blanca, Mexico, Nopal I ore deposit (black), altered rock (gray), and proposed borehole locations (red). Heavy black lettered lines are fractures

O.2 Bangombé

Statement of Problem

A better understanding is needed of the upper bound of mobility of uranium and fission products in the unsaturated zone (UZ) at Yucca Mountain under higher infiltration flux.

Impact/Importance to Yucca Mountain Project

This work will provide an estimate of radionuclide transport under reducing and oxidizing conditions at the same site, and the relative contribution of each to overall radionuclide migration under conditions of higher infiltration flux than at Yucca Mountain. While the UZ at Yucca Mountain is believed to have prevailing oxidizing conditions, the available data do not preclude the existence of reducing conditions in sealed drifts or in zones with oxygen displaced by water vapor.

Objective

The primary objective is to use radionuclide transport information from the Bangombé reactor near Oklo, Gabon as an end member to understand the range of migration/sequestration behavior of uranium and its daughter products under reducing and oxidizing conditions, both of which are found in the Bangombé natural system. This information will be used to provide confidence in the long-term sequestration of spent fuel over a range of environmental conditions at the proposed Yucca Mountain repository. This information will provide corroborating data for flow and transport models in the UZ.

Workscope

The Bangombé natural reactor in Gabon is located in unsaturated clays and sandstones and underwent fission approximately 2 billion years ago. Since then the system has been open to the influx of water and the migration of uranium and its daughter products through unsaturated flow and transport (Figure O-2). In contrast, the uranium deposit at Peña Blanca, Mexico (Proposal O-1) appears to have been a system closed to the migration of uranium for at least the last 300,000 years (CRWMS M&O 2000a). Thus, the two deposits may provide bounding data regarding stability of uranium and its daughter products, as analogues to spent fuel, over a range of environmental conditions. Because the Bangombé site is located at a very shallow depth (12 m from the surface; Del Nero et al. 1999), the natural reactor at Bangombé is of particular interest to elucidate the role of present-day weathering in the partition of uranium and fission products (Salah 2000).

The information obtained from this study can be used to understand and predict the mobility (or retardation) of radioactive contaminants under conditions and time scales relevant to long term isolation of high-level waste at Yucca Mountain. For example, uranium is itself of concern and is also geochemically similar to some transuranic elements, e.g., neptunium; Th (IV) can be used as a proxy for Pu (IV), Pa (V) for Pu (V), etc. The transport rate of ^{137}Cs, ^{90}Sr and ^{133}Ba can be inferred from that of ^{226}Ra, provided that the geochemical fractionation between Cs, Sr, Ba and Ra can be reasonably determined by measuring their concentrations in fluid and rock samples. The natural analogue approach has advantages over laboratory studies and theoretical calculations in that the natural analogue approach takes into account the combined effects of variable speciation, geologic heterogeneity and geologic time scales. The role of processes such as colloidal transport of uranium-series elements and the role of matrix diffusion in retarding them will also be investigated.

Tasks

1. Summarize available information in literature on Bangombé reactors. Determine representative number of samples required and sample locations.

2. Obtain core samples from University of Michigan.

3. Determine need for additional characterization of secondary minerals and characterize, if needed. Provide description of secondary mineralization.

4. Conduct uranium-series isotopic characterization on selected samples.

5. Working with Université Louis Pasteur, Strasbourg, investigate possibility of obtaining new water samples; prepare plan for obtaining samples in future.

6. Preliminary modeling of solid phase data and application to numerical models of UZ flow and transport at Yucca Mountain.

7. Incorporate new data from water samples (dependent on Task 5) or use existing hydrochemical data in UZ flow and transport model.

8. Prepare final report on Bangombé as an end member scenario for open-system transport of uranium in the UZ at Yucca Mountain.

Schedule

Year 1: Tasks 1-5

Year 2: Task 6-8

Products

Annual progress reports will be made to DOE on results of the study. The work will provide a contribution to update of *Natural Analogue Synthesis Report* (see Proposal O-1). One peer-reviewed publication will be submitted on the results of the study.

Level of Effort

Task	Year 1	Year 2
1 and 2	$^1/_3$ FTE	—
3	¼ FTE	—
4	$^2/_3$ FTE	$^1/_3$ FTE
5	¼ FTE	—
6	—	$^1/_3$ FTE
7	—	$^1/_3$ FTE
8	—	$^1/_3$ FTE

Principal Investigator – uranium isotope series analyses, development of conceptual model

Modeler – numerical model

Analysts – chemical analysis of waters and isotopic analyses

Geologist/mineralogist – secondary mineral analysis

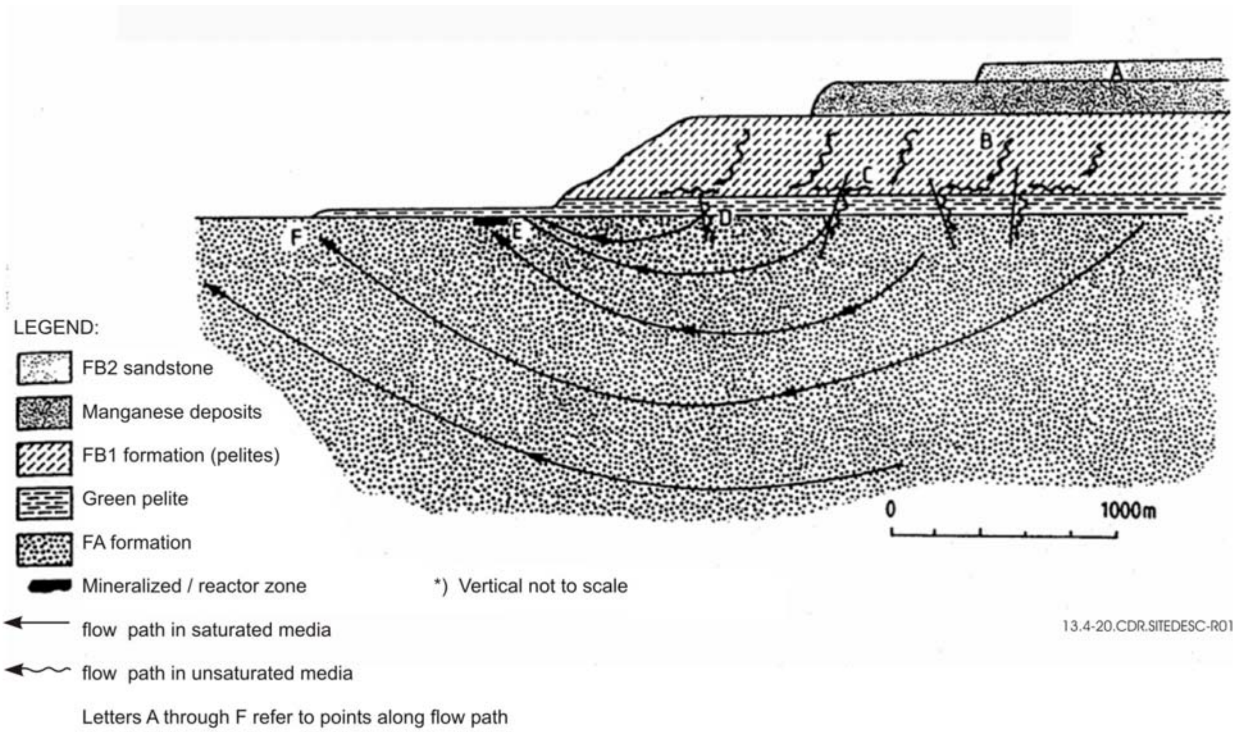


Figure O.2 Schematic representation of groundwater flow paths in the Bangombé area. (CRWMS M&O 2000b, Fig. 13.4-20).

O.3. Site-Scale Model of Rainier Mesa

Statement of Problem

Numerical models of UZ flow and transport at Yucca Mountain require validation by testing their ability to replicate flow and transport conditions at field sites.

Impact/Importance to Yucca Mountain Project

The proposed work has significant potential for improving confidence in UZ flow and transport models because of the similarity between Rainier Mesa and Yucca Mountain in terms of hydrogeologic properties. Rainier Mesa , located in close geographic proximity to Yucca Mountain but at higher elevations with higher precipitation, is a good analogue for UZ processes under future wetter climate conditions. The extensive tunnel complexes, excavated decades ago, have collected hydrologic and transport data to characterize the test beds for underground nuclear testing (see Figure O-3). Most of the tunnels have since been sealed, but are monitored with sensors to measure the seepage and accumulation of water behind bulkheads. This information will be valuable for Yucca Mountain before similar extensive tunnel complexes are excavated for repository drifts. Performance confirmation approaches can then be developed from this analogue knowledge.

Workscope

It is assumed that data sets can be obtained from unclassified sources for constructing the Rainier Mesa hydrogeologic model. Data will be obtained from the NTS on borehole lithology, hydrology, surface topography, precipitation, and infiltration, and other available data. The data will be used to formulate a conceptual model of flow from Rainier Mesa to areas of discharge. A three-dimensional, site-scale grid will be constructed over a surface area of several km (to be determined). The suite of numerical tools used in the Yucca Mountain site-scale model of UZ flow and transport will be used to model flow and transport in the Rainier Mesa area, possibly including evaluation of drift shadow effects. Results of the Rainier Mesa numerical model will be compared to field data and conceptual models. Then, using the same limited sets of data but with Yucca Mountain data, the UZ flow and transport model will be run to see whether the same results are obtained with limited data as with the full complement of site characterization data available for the UZ. This provides a measure of model validation as well as of verification.

Schedule

Year 1: Obtain data and build Rainier Mesa conceptual and numerical models. Run numerical model and compare model results to measured field observations.

Year 2 : Run UZ flow and transport models for Yucca Mountain using exclusively the same types of data sets as used in the Rainier Mesa model. Compare to results of UZ flow and transport models that use more extensive data sets to see whether the more extensive data sets are required to produce realistic results that agree with observations. Document results of study and relevance to model confidence-building in products below.

Product

Contribution to update of *Natural Analogue Synthesis Report* (see Proposal O-1); peer-reviewed publication. Contribute to annual report of progress to DOE.

Level of Effort

Year 1: 1 FTE
Year 2: 1.5 FTE

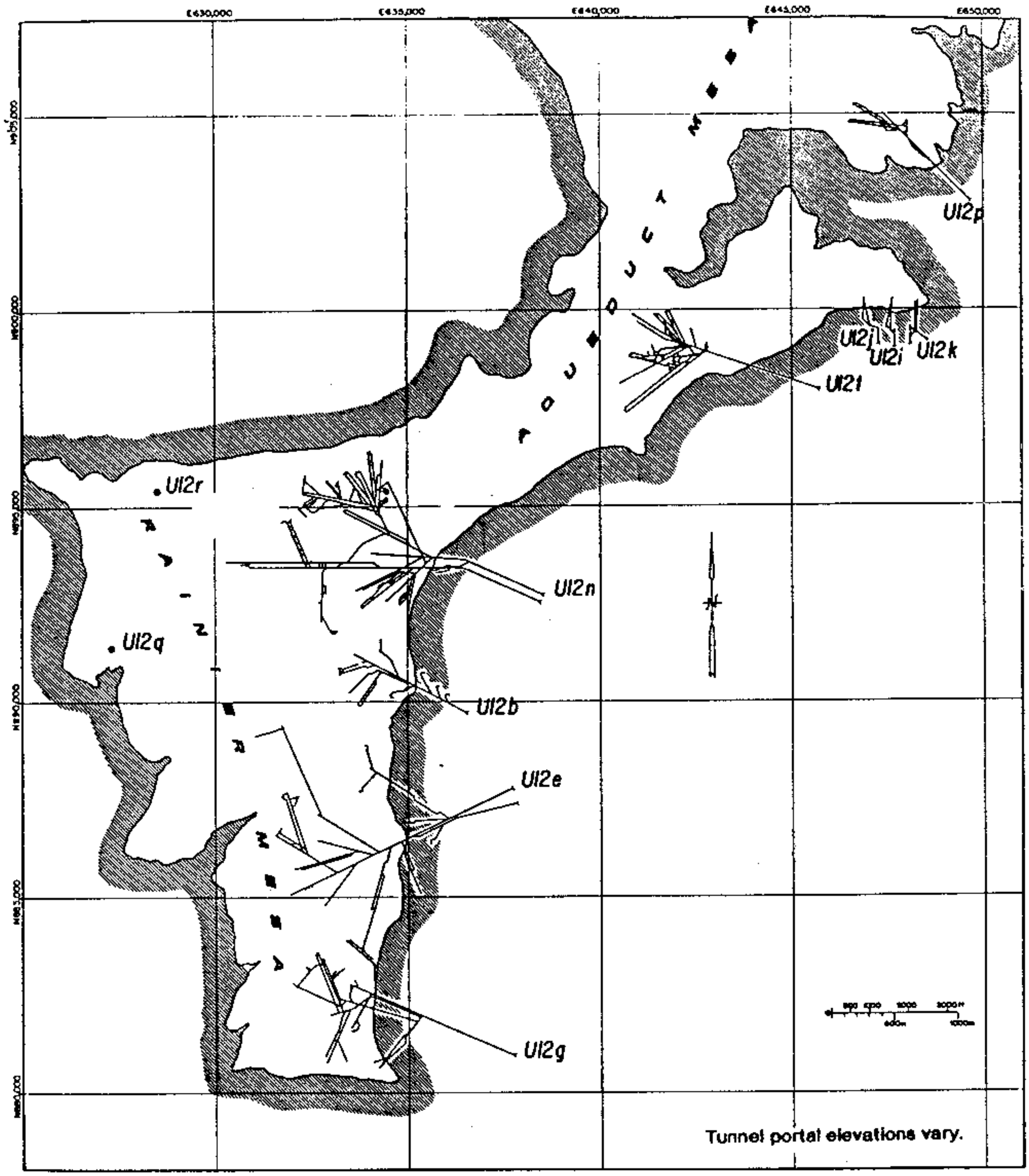


Figure O-3. Reference map of Rainier and Aqueduct mesas showing locations of tunnel complexes (Wang 1991, after Defense Nuclear Agency 1989).

O.4. Drift Shadow Analogues

Statement of Problem

Models of flow and transport beneath the drift do not reflect the presence of a drift shadow (Philip et al. 1989). This may lend unnecessary conservatism to unsaturated zone (UZ) models.

Impact/Importance to Yucca Mountain Project

Incorporation of the drift shadow into UZ flow and transport models has the potential for increasing the robustness of the natural barrier by several orders of magnitude. In order to verify the presence and efficacy of the drift shadow, it needs to be tested in natural and anthropogenic underground openings that have not been disturbed in recent decades by artificial introduction of water (see also Proposal H).

Objective

The purpose of this natural-analogue study is to investigate settings having the potential to demonstrate efficacy of the drift-shadow zone in diverting flow beneath the repository. Suitable natural and anthropogenic analogue sites will be selected for testing the drift shadow zone concept through drilling and monitoring moisture. This work will design the first test, construct the test, instrument boreholes, collect data and begin analyses. It will select a location for a second test. Locations for further investigation of test feasibility include, but are not limited to, Hoover Dam tunnels, Apache Leap tunnel, caves and mines, Rainier Mesa tunnels, Hanford Tanks. The work will incorporate knowledge gained from these tests into corroborative information to be used in validation of the UZ flow and transport models.

Work Scope

A predicted consequence of the preferential diversion of water around underground openings is the development of a dry-out zone beneath the opening. Such a zone beneath stored waste would function as an additional impediment to the mobilization of radioactive material towards the accessible environment. Unfortunately, this postulate can not be accurately tested in the underground facility at Yucca Mountain because the natural system has been greatly perturbed by the heavy use of construction water for dust control and by the large volumes of air exhausted every day. Furthermore, there has probably not been enough time for the underground facility to come to equilibrium with the undisturbed host rock.

Naturally occurring caves provide an opportunity to test for the presence of a dry-out zone beneath an opening in the unsaturated zone. Both limestone and gypsum caves would be hydrologically similar to the welded tuffs at Yucca Mountain because in both cases flow would occur primarily along fractures. Furthermore, caves would have had sufficient time to establish hydrologic equilibrium. The large number of caves in the Carlsbad, New Mexico region would allow choosing a cave that closely matches the physical characteristics of a potential mined geologic repository and avoiding potentially complicating features, as described above. Caves that are known to receive direct surficial runoff should be eliminated from consideration. The cave chosen for study should be as large as or larger than proposed repository emplacement drift cross sections, currently approximately 5 m in diameter. The roof of the cave should be below the zone of surface influence, currently estimated as 6 m. Ideally, the cave should be readily accessible to light drilling equipment, but not generally in use by the public who might disturb sensitive scientific equipment and site conditions. The cave should be sited so as to accommodate a small meteorological data station or be close to an area where such data are currently being collected.

The cave study will be planned to accommodate two phases. The first phase requires coring two small diameter drillholes (approximately 1.5 cm diameter). One would be drilled horizontally a short distance into the wall of the cave. The core would be analyzed for hydrologic properties and the hole would be instrumented with lysimeters for approximately 2 years to monitor moisture content. A second hole would be drilled in the floor of the cave. The actual depth would be established by model results for the chosen cave, but the anticipated depth would be less than 30 m. The core from the second hole would be analyzed for moisture content, and the hole would be instrumented and monitored for 2 years.

The site chosen should be amenable for standard tracer or infiltration tests in the event that the results of the first phase of the experiment suggest that results from further experimentation would be useful. The infiltration tests would push the system out of hydrologic equilibrium by applying enough water to the surface above the cave to establish dripping into the cave. The tracers would be dyes or biodegradable tracers that would be used in an attempt to define flow paths. Two sites, one natural and one anthropogenic, are provided as examples.

Boyd's Waterhole

The small cave approximately 800 m southeast of Boyd's Waterhole appears to meet the necessary criteria. The cave and waterhole are located in township T22S, range R25E on the Azotea Peak 1:24,000 quadrangle, New Mexico. The cave shows signs of occasional recreational use, and is therefore, unlikely to be found of archaeologic value. The cave is less than 100 m off the road, and therefore, a portable drill could easily be carried to the cave by two persons. Holes will be dry-drilled to minimize the impact of water on the cave environment. It is anticipated that each hole could be drilled in a day.

Hoover Dam

The Tunnel Plug Access Tunnel on the Arizona side of Hoover Dam was selected as a promising location for testing the drift shadow zone concept in an anthropogenic setting. The tunnel has a one-foot-thick lining of concrete and is approximately 10 feet in diameter. In Figure O-4, this tunnel is shown by "×". It sits 5 feet above the Colorado River.

The plan is to drill three angled holes. The first can be drilled from a point 5 m in front of the tunnel entrance and would angle below the tunnel to where it would become horizontal. The second and third angled holes can be drilled 5 m away from the first hole on either side of the tunnel. The drillholes will be instrumented with removable resistivity probes located at periodic intervals along their length. The probes will measure changes in moisture content that could detect passage of a wetting front. These will be monitored after precipitation events. In theory, if the tunnel is not located where the water table has been disturbed by the location of the dam (this will first need to be determined), the probe beneath the tunnel should not experience passage of a wetting front, whereas the probes along either side of the tunnel should. Monitoring would take place for a minimum of 2 years. During the second year of the test, an option for chemical sampling *in situ* using fiber optic methods will be explored. The purpose of chemical sampling is to detect differences in chemical signature of infiltrating meteoric water below and lateral to the tunnel.

Information from the drift shadow tests will be used as modeling input in conjunction with Proposal H. See Proposal H for details of modeling.

Schedule

Year 1: Investigate DSZ test locations, plan DSZ tests, perform first DSZ test, analyze and interpret first test results

Year 2 Conduct tests in second location, analyze and interpret results of second test, incorporate results of both sets of tests into UZ flow and transport model for model validation

Year 3: Prepare updated results of DSZ model for publication

Product

Results of these tests and models will be incorporated into an update of the *Natural Analog Synthesis Report*, TDR-NBS-GS-000027, and in peer-reviewed publications. An annual progress report will also be provided to DOE.

Level of Effort

Year 1: 1.7 FTE

Year 2: 2 FTE

Year 3: ½ FTE

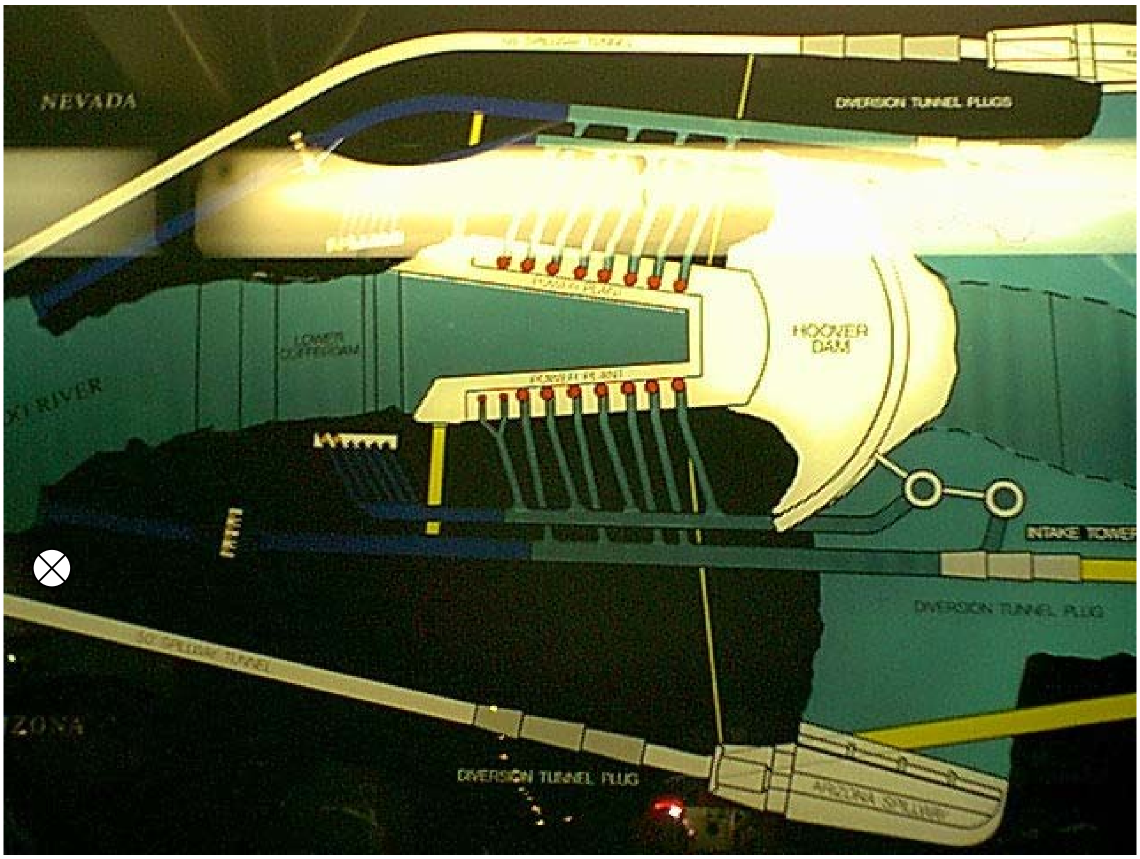


Figure O-4. Map of Hoover Dam showing penstocks and tunnels (from a photograph, not to scale).

O.5. Alternate Transport Analogue Site

Statement of Problem

1. Schedule delays at Peña Blanca, the preferred analogue site, may drag on indefinitely and may compromise the ability to build confidence in UZ transport models through natural analogues. For this reason, it would be wise to select an alternative site or sites for study that do not have the same access problem.

2. Other process models discussed in the *Natural Analogue Synthesis Report* (BSC 2001) have not been validated using natural analogues to the extent that they might be used beneficially. Models of saturated zone (SZ) transport in alluvium, stability of drifts, waste package corrosion, and igneous intrusion into a repository-like setting could build confidence through use of natural analogues.

Impact/Importance to Yucca Mountain Project

Process models will benefit by being exercised with carefully chosen data sets and conceptual models based on natural analogue sites. Use of natural analogues for this purpose also has the potential for increasing public confidence that the correct processes have been incorporated into models and that the models have reasonable parameter bounds.

Objective

The primary objective in Year 1 is to locate a site with favorable features and conditions that could serve as a backup replacement for testing at Peña Blanca, in the event that drilling cannot be accomplished in Mexico. The backup site could be located in the western United States (e.g., northern Nevada [see CRWMS M&O 2000a], Arizona, New Mexico) (Figure O-5) or could involve collaboration with institutes in a foreign country where that country collects the data and provides it to the Yucca Mountain Project (YMP). An example is a uranium mine in the southern Caucusus in Russia (currently studied by DOE investigators in cooperation with the Russian Academy of Sciences) or other sites in Russia. Once the site location and screening are performed, the objectives would be the same as those expounded upon in Proposal O.1.

A second objective is to use this proposal as a placeholder for potentially beneficial studies that could be conducted to support other process models (note: not having seen proposals from groups outside LBNL, we don't know whether natural analogues have been incorporated into work in the other focus areas). This proposal provides a placeholder for analogue studies in other focus areas, because we believe that natural analogues (including anthropogenic analogues) are useful for building confidence in all types of process models.

Workscope

For the UZ transport alternate analogue, several alternate candidate sites will be investigated for studying UZ transport in the first quarter of the year. A written analysis will be provided of their advantages, disadvantages, existing background information, and data gaps. Sites will be prioritized for study and recommendations will be mde for adoption by YMP, in the event that the Peña Blanca study doesn't work out. In second quarter, plans will be written for an alternate transport site study. In third quarter, researchers will begin to work on the plan. The workscope cannot be specified further at this time, but would be developed to construct a three-dimensional model of UZ transport at the analogue site, similar to workscope and objectives for Peña Blanca study (see Proposal O-1). In the second year, additional data collection might take place and the majority of the modeling and interpretation with respect to Yucca Mountain long-term performance would be performed.

For the analogues in focus areas not related to UZ transport, workscope would be provided later in Year 1 of the alternative transport analogue investigation.

Schedule

(Explained to the degree possible in workscope above)

Level of Effort

Year 1: 1 ¼ FTE for UZ transport alternative analogue (no work on other focus areas)

Year 2: 1 FTE for UZ transport alternative analogue (FTEs for other focus areas would be determined during first year)

Product

Results of these tests and models will be incorporated into an update of the *Natural Analog Synthesis Report*, (BSC 2002) and in peer-reviewed publications. An annual progress report will also be provided to DOE.

References for Proposals O.1-O.5

BSC (Bechtel SAIC Company) 2002.*Natural Analogue Synthesis Report.* TDR-NBS-GS-00027 Rev 00 ICN02. Las Vegas, Nevada: BSC.

BSC 2001. Site Investigation Test Plan (SITP) for Natural Analogues. SITP-02-NA-001, Rev. 00.

Castor, S.B., Henry, C.D., and Shevenell, L.A., 1996. *Volcanic Rock-Hosted Uranium Deposits in Northwestern Nevada and Southeastern Oregon - Possible Sites for Studies of Natural Analogues for the Potential High-Level Nuclear Waste Repository at Yucca Mountain, Nevada.* Report from Mackey School of Mines, Reno, Nevada: University of Nevada. ACC: MOL.19960927.0026.

CRWMS M&O 2000. *Natural Analogues for the Unsaturated Zone*. ANL-NBS-HS-000007 Rev00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL 19990721.0524.

CRWMS M&O 2000b. *Yucca Mountain Site Description.* TDR-CRW-GS-000001, Rev 01 ICN 01. Las Vegas, Nevada: CRWMS M&O.

Del Nero, M., Salah, S., Miura, T., Clément, A., and F. Gauthier-Lafaye, 1999. Sorption/desorption processes of uranium in clayey samples of the Bangombé natural reactor zone, Gabon, *Radiochimica Acta* 87, pp. 135-149.

Philip, J.R.; Knight, J.H.; and Waechter, R.T. 1989. Unsaturated Seepage and Subterranean Holes: Conspectus, and Exclusion Problem for Circular Cylindrical Cavities.: *Water Resources Research, 25* (1), 16-28. Washington, D.C.: American Geophysical Union.

Salah, S., 2000. Weathering processes at the natural nuclear reactor of Bangombé, Gabon. Identification and geochemical modeling of the retention and migration mechanisms of uranium and rare earth elements. Unpublished doctoral dissertation, Université Louis Pasteur, Strasbourg, 256 pp.

Wang, J.S.Y. 1991. Propagation of infiltration pulses through unsaturated tuff units. In *A Review of Rainier Mesa Tunnel and Borehole Data and Their Possible Implications to Yucca Mountain Site Study Plans.* LBL-32068. Berkeley, California: Lawrence Berkeley National Laboratory.

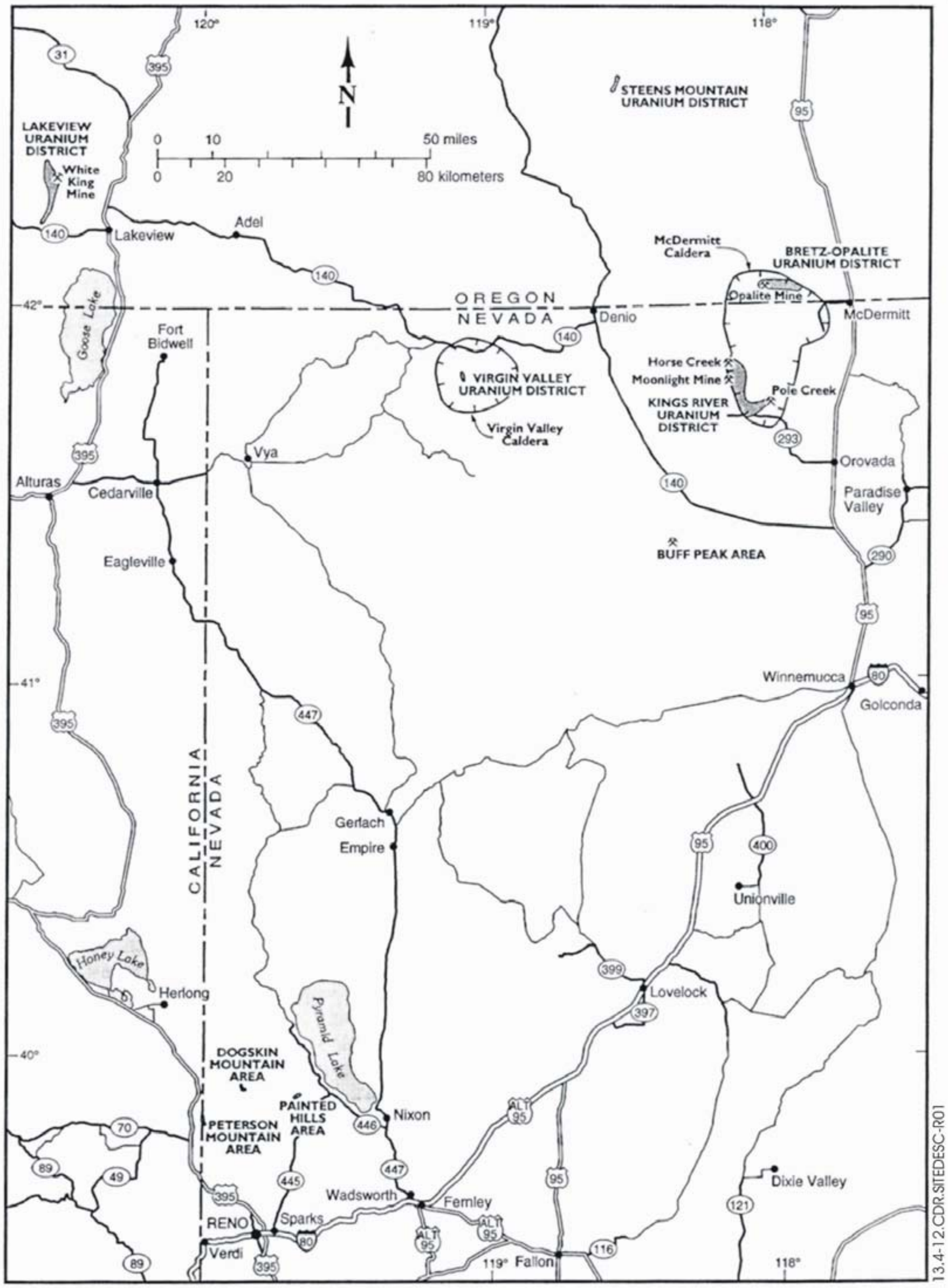


Figure O-5. Location of uranium districts in northwestern Nevada and southeastern Oregon that may be suitable for an alternate transport analogue study (from Castor et al. 1996)

P. Building Confidence in Nuclear Waste Isolation and Safety through International Collaboration

Focus Area: International
Contact: A. Simmons, AMSimmons@lbl.gov, (510) 486-7106
Collaboration: LBNL, LANL, LLNL, SNL, USGS

Statement of Problem

More than fifty nations around the world face the issue of radioactive waste disposal, whether or not they use nuclear power to generate electricity. The global consensus is that the safest means of disposal of high-level waste is deep underground in a stable geologic environment. Some nations have studied a variety of candidate areas and sites within their borders for over a decade; other nations are just beginning the site screening process. All national programs face both technologic and societal challenges to their waste disposal solutions. These challenges can be met more effectively by collaborating with other countries who are working on the same problem and building upon the lessons learned by others.

Impact/Importance to Yucca Mountain Project

The United States leads other countries in nuclear waste disposal in being the first nation to construct an underground repository for transuranic waste at the Waste Isolation Pilot Plant. Other nations view the U.S. in the forefront of high-level nuclear waste disposal also. International collaboration has the potential to strengthen public acceptance of geologic disposal as a disposal solution for nuclear waste in the U.S. The transfer of technologies among nations, collaborative testing, and model validation exercises also increase the probability of arriving at defensible models and safe repository designs. A major benefit is having DOE's scientific work independently reviewed, replicated, critiqued, and hence, strengthened at very little additional cost. Results of this work will be useful to waste disposal programs in other countries and will be made available through the LBNL International Center.

Objective

International collaboration has several purposes and benefits. First, international collaboration in the following proposed tasks can demonstrate the knowledge and experience gained in the U.S. program over decades and can provide training for other nuclear waste programs, resulting in a wide distribution of technology transfer. Second, international collaboration provides additional opportunities to test and validate conceptual and numerical models at different scales and in different settings. This builds confidence in the models across the scientific community that can be communicated to increase public acceptance.

Workscope

1. LBNL International Center for Radioactive Waste Disposal

   - Training center – The center will serve as a training ground for scientists, regulators, and decision-makers from other countries in the realm of nuclear waste disposal. The center will also use existing facilities and numerical modeling tools for visiting researchers who are working on flow and transport experiments related to contaminated waste sites and nuclear waste disposal.
   - Collaborative experiments – The center will work with waste disposal programs in other countries to identify research topics that would benefit by collaborative experiments of U.S. researchers in underground research laboratories or field sites in other nations or international researchers working in the ESF. (The existing arrangement between DOE and AECL is a good example of the type of projects, but differs contractually from the center concept).
   - Public acceptance – involve local scientists who focus on risk reduction issues to investigate successful approaches to gaining public acceptance for nuclear waste facilities, focusing particularly on waste disposal. Examine approaches taken successfully by other countries and the reasons for success, as well as the reasons for failed approaches. Develop a plan for improving public acceptance

in the U.S. through multiple avenues that reduce the perception of risk among the many varied sectors of the population.

2. DECOVALEX – participate on steering committee for continuation phase of DECOVALEX.

   DECOVALEX is an international consortium of agencies (governmental and non-governmental) associated with the disposal of nuclear waste. The mission of DECOVALEX is **DE**velopment of **CO**upled models and their **VAL**idation against **Ex**periments. The current/third project started in 1999 and is scheduled to conclude in October 2003. The DOE joined DECOVALEX III with the Drift-Scale Test as one of the experiments used for coupled process model validation. The NRC is also a participant in DECOVALEX III. Currently, Canada, France, Finland, Germany, Japan, Spain, Sweden, United Kingdom, and the U.S. are represented in DECOVALEX**.**

   There are four tasks in DECOVALEX III, as follows. The DOE is a participant in Task 1 and Task 3BMT2 and the lead for Task 2. DOE investigators perform the calculations, modeling, analyses, and investigations associated with Task 1 and Task 3BMT2. These activities for Task 2 have already been completed by DOE, so that current DOE tasks involve only co-ordination and documentation. The planned DECOVALEX activities in FY03 are:

   Task 1: Complete and document the modeling of THM response in the FEBEX test, a full-scale engineered barrier system test being conducted at the Grimsel site in Switzerland.

   Task 2: Yucca Mountain Drift Scale Test. Coordinate all activities; model and analyse the THM response of the Drift-Scale Test; and prepare the Task 2A (TH), Task 2B/C (THM), and Task 2D (THC) reports.

   Task 3: Model/calculate the effect of homogenization on the performance of a hypothetical repository and prepare report. Task 3 has three sub-tasks: BMT1 on resaturation, BMT2 on homogenization or upscaling, and BMT3 on glaciation.

   Task 4: Survey and document the extent of application of coupled process modeling in the total system performance assessments (TSPA)s of various programs.

   A task should be added to develop Phase IV of DECOVALEX, placing more emphasis on the models.

3. Transport analogue sites in Russia

   Actinide speciation and transport data from Russian anthropogenic analogue sites can provide valuable corroboration of transport data, calculations, and transport models that provide input to total system performance assessments (TSPAs). The concentration of mobilized actinides at the surface of exposed waste forms and their chemical speciation during transport are important uncertainties that are treated in a bounding fashion in current YMP analyses. Environmental analogue data, along with laboratory data and process modeling, are components of the approach to developing more accurate representations with narrower bounds. A number of contaminated sites and/or disposal facilities in Russia (e.g., Mayak, Tomsk, Krasnoyarsk) will be studied in this proposed task as potential analogues for speciation, complexing, and migration or sequestration of radionuclides in deep geologic environments. Using data previously collected by Russian investigators, thermodynamic and kinetic parameters will be calculated, including diffusion coefficients, complexation strength of different ligands with actinides, and the chemical composition of soluble actinide species and colloids in natural waters. The determined parameters will then be used to test conceptual and numerical models of transport at the Russian sites and will be further used to provide realistic parameter bounds in transport models applied to Yucca Mountain.

4. Colloids

   DOE researchers already participate in the Grimsel, Switzerland tests on colloid transport in granodiorite. However, it remains to be seen how far in distance colloids can be transported in a saturated environment such as Grimsel and how results of the Grimsel colloid test can be applied to transport in an unsaturated environment. The Grimsel colloid test also provides necessary data on colloid origin, size, and composition that will provide the necessary parameters for testing colloid transport models.

Schedule

	Year 1	Year 2	Year 3	Year 4	Year 5
1. International Center					
Training Center	●	●	●	●	●
Collaborative Experiments		●	●	●	●
Risk reduction and public acceptance projects	●	●	●	●	●
2. DECOVALEX	●	●			
3. Russian Analogue sites	●	●	●		
4. Colloids at Grimsel	●	●	●		

Products

All tasks will provide annual progress reports to DOE. Papers will be written for presentation at international conferences and meetings. One or more peer-reviewed journal articles will be submitted for each of Tasks 1, 3, 4, and 5. In addition, the International Center will sponsor an international workshop tri-annually, similar to those organized by Paul Witherspoon of LBNL on "Challenges in Geologic Disposal of Radioactive Waste". The workshop will provide a forum for sharing results of progress of the International Center and will provide updates from countries around the world on their ongoing efforts in radioactive waste disposal. Workshop proceedings will be published by LBNL.

Level of Effort

	FY 1	FY 2	FY 3	FY 4	FY 5
1. International Center					
Training Center	1 FTE	1 FTE	1 FTE	1 FTE	1 FTE
Collaborative Experiments		2 FTE	2 FTE	2 FTE	2 FTE
Risk reduction and public acceptance projects	1 FTE	1 FTE	1 FTE	1 FTE	1 FTE
2. DECOVALEX	1.5 FTE	1.5 FTE			
3. Russian Analogue sites	0.5 FTE	1.25 FTE	0.75 FTE		
4. Colloids at Grimsel	0.5 FTE	0.5 FTE	0.5 FTE		

APPENDIX. Overview of LBNL Science Proposals

Editor's Note: The following presentation was given as an overview to the LBNL science proposals on August 15, 2002, in a meeting with Mr. Stephan Brocoum and Mr. Dennis Williams from the DOE/LV Science and Technology Program. Since then, modifications were made to some of the proposals, one proposal was deleted, and the order was changed slightly. These modifications explain the absence of a one-to-one correlation between proposals in this booklet and the form in which they were presented in August 2002.

Overview of LBNL Science Proposals

Bo Bodvarsson, Lab Lead

August 15, 2002

New Direction for Cost Reduction

- Cut the cost by $10 billion from the current Total System Life Cycle Cost estimate of $58 billion
- Find cost savings in "very expensive engineering" such as waste packages and "drip shields"
- "Regardless of the budget, there will be a science and technology program. I'll make it happen."

Margaret S. Y. Chu

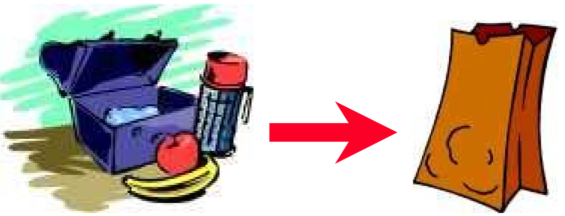
Director of DOE OCRWM

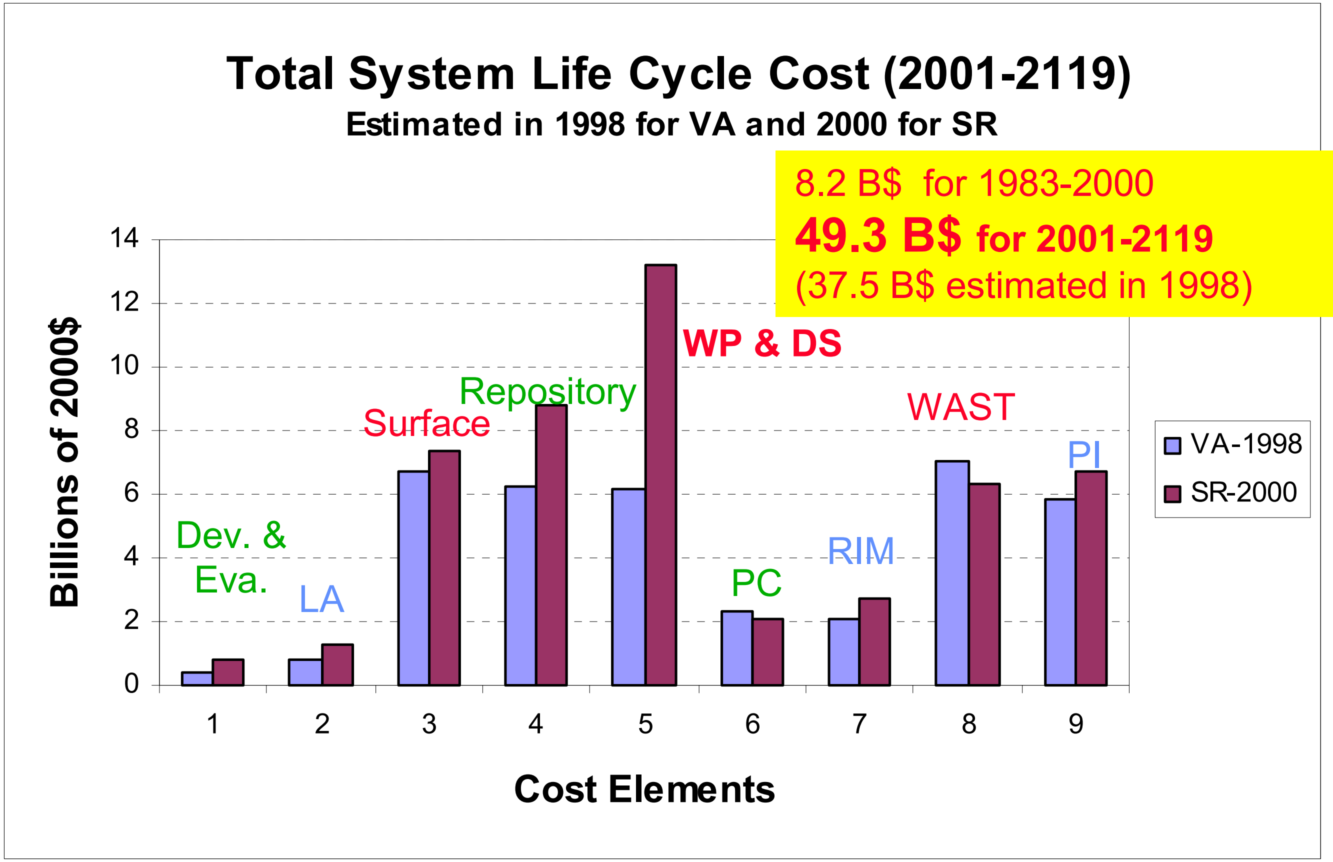
speaking at a meeting of the
National Academy of Sciences'
Board of Radioactive Waste Management

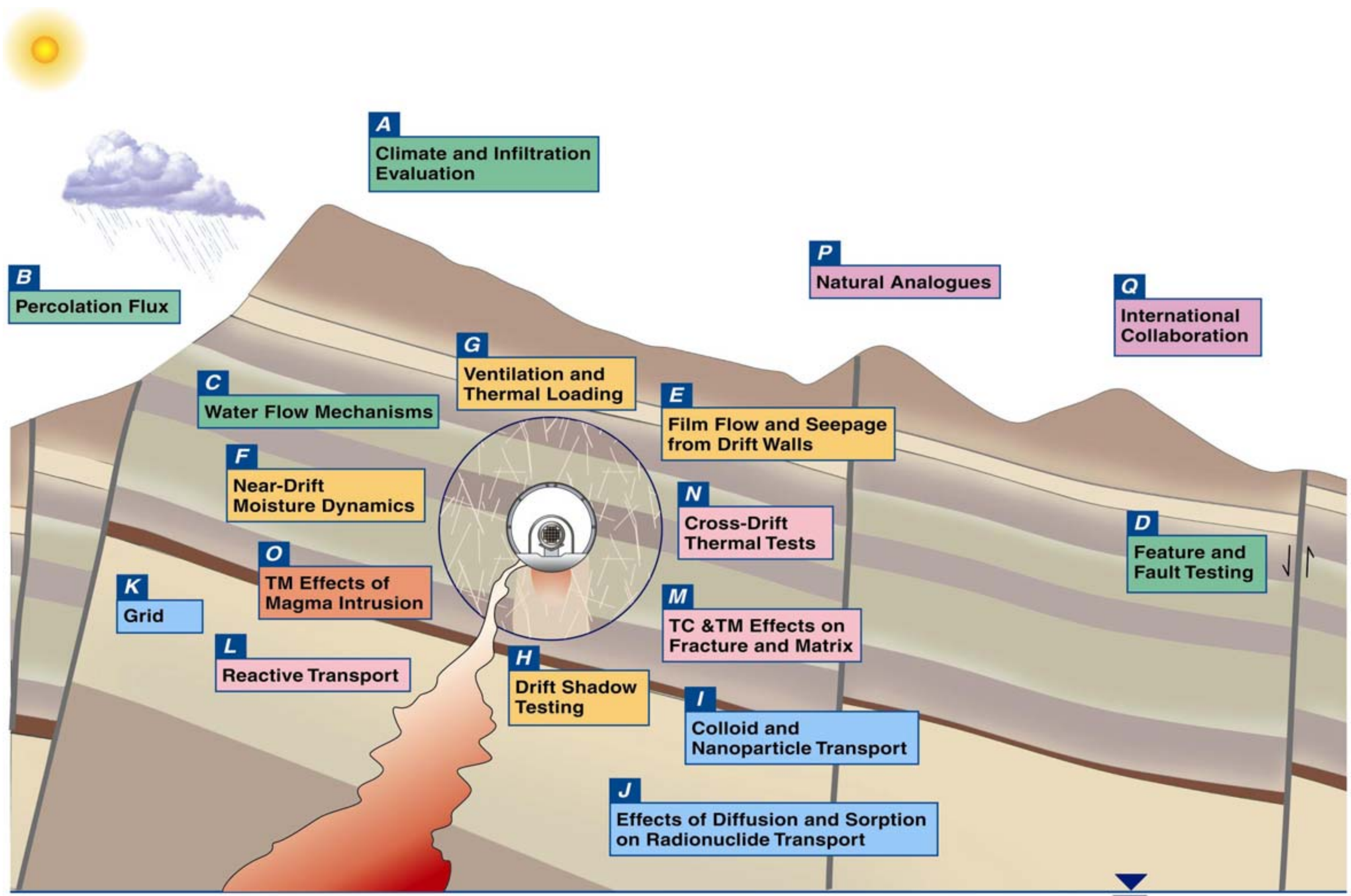
- Currents, August 9, 2002

Total System Life Cycle Cost Reduction

- Natural Barriers (including man-made drifts) can be optimized to supplement or replace redundant engineered components
- Potential Cost Reduction with refocusing on Natural Barrier performance







Not to Scale

NW02-015

Proposals to Enhance Natural Barrier Performance

A: Miller, climate
B: Dobson, geochem
C: Birkholzer, focusing
D: Wang, fault
E: Tokunaga, film
F: Salve, in-drift
G: Unger, ventilation
H: Houseworth, shadow
I: Wan, colloid
J: Max: diffusion
K: Pruss, grid
L: Sonnenthal, reactive transport
M: Kneafsey, THC/M
N: Tsang, CDTT
O: Oldenburg, magma
P: Simmons, NA
Q: Simmons, International

Focus Areas

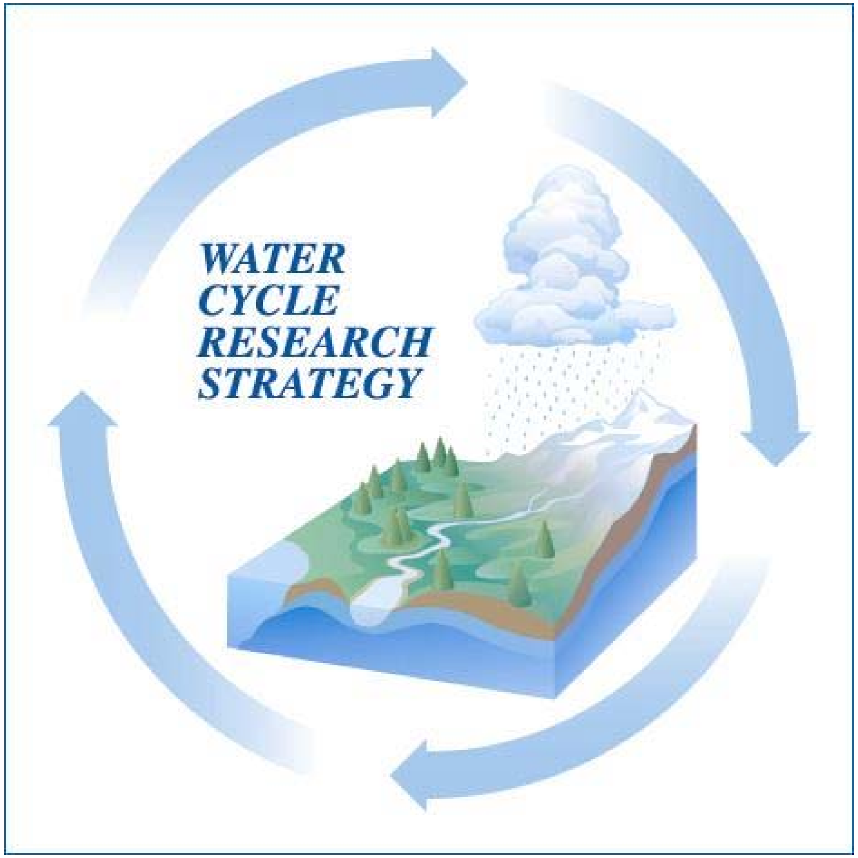
- UZ Flow
- Man-Made Natural Barriers
- UZ Transport
- Coupled Processes
- Volcanism
- Natural Analogues / International Collaboration

Focus Areas

- UZ Flow: Reduce Uncertainties in (A) Greenhouse effect, (B) Overestimation of Percolation Flux, (C) Flow Focusing, and (D) Fault Channeling.
- Man-Made Natural Barriers
- UZ Transport
- Coupled Processes
- Volcanism
- Natural Analogues / International Collaboration

Nested Global to Site-Scale Modeling of Climate/Infiltration

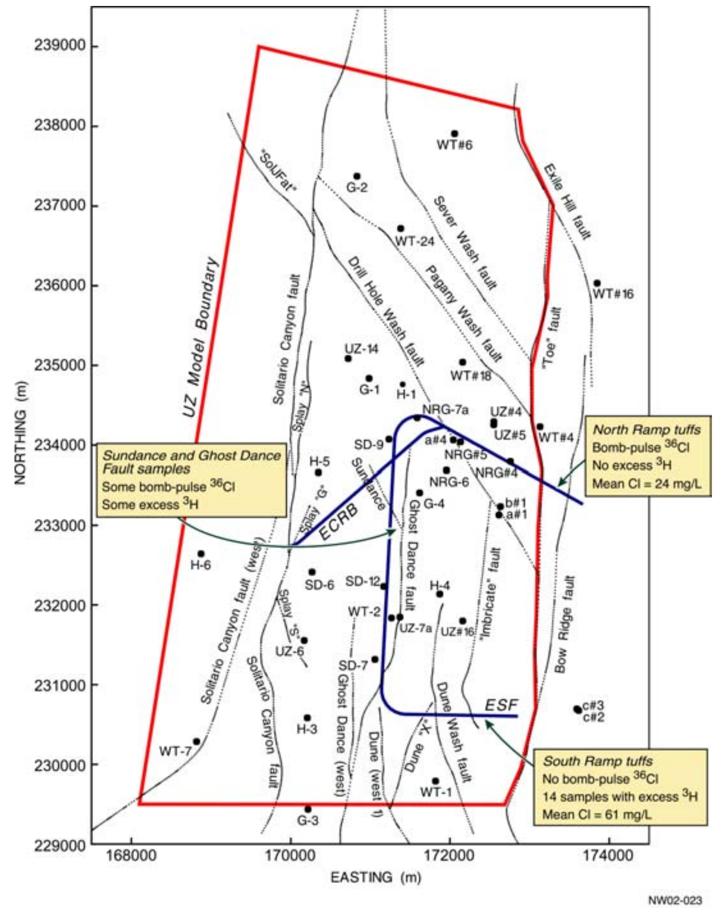
- Apply realistic representation with physically-based model to address greenhouse effects
- Determine the likelihood for current models in grossly over (or under) estimating climate/infiltration
- Reduce uncertainties (current climate is monsoon or dry ?)



Climate and Infiltration Evaluation with Nested Modeling from Global to Site-Scale at Yucca Mountain - N.L. Miller et al.

Bounding Percolation Rates with Geochemical Data

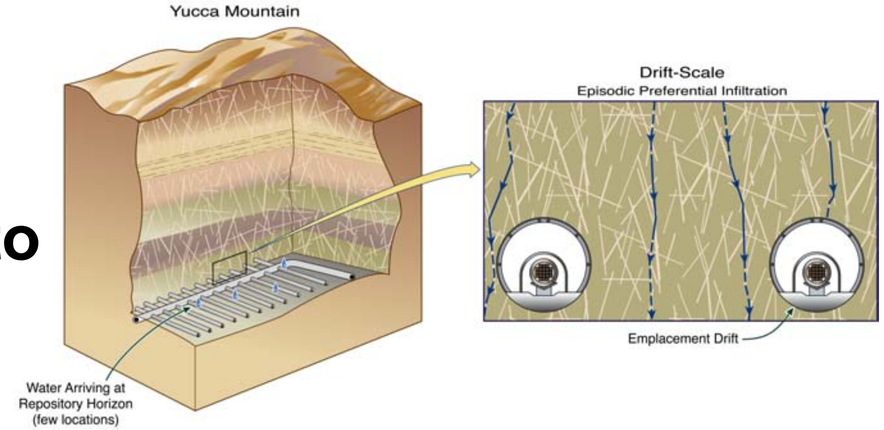
- **Use all available geochemical data (Sr, calcite, U, etc.) to constrain the flow field, based on extension of total chloride balance approach**
- **Determine if the percolation is overestimated from (e.g. ~6 mm/yr over tens of thousands of years)**
- **Quantify chemical heterogeneity in assessing waste package corrosion**



Application of Geochemical Data to Bound Current and Past percolation Rates - P.F. Dobson et al.

Flow Focusing from Pore-Scale to Drift- and Site-Scales

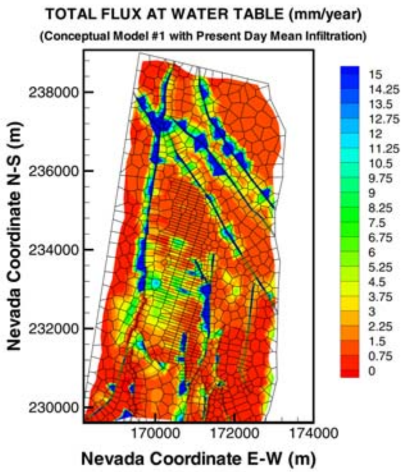
- Determine the spacing between active flow paths similar to the only feature observed during niche excavation
- Quantify the localized flux in determining seepage into drifts under both ambient and thermal conditions
- Evaluate if the fracture flow at YM episodic and preferential

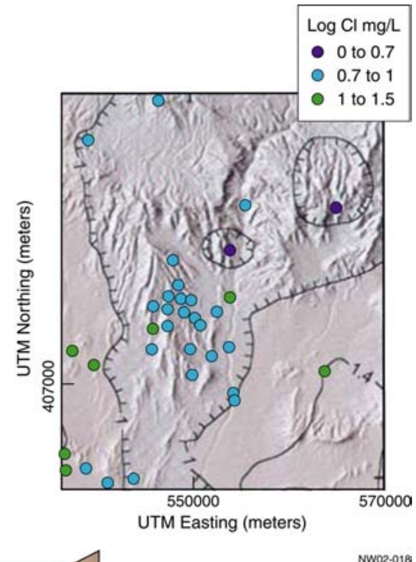


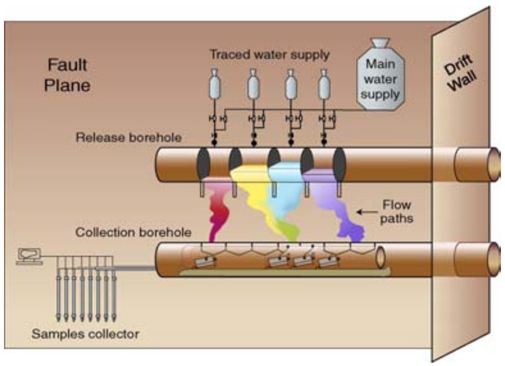
Water Flow Mechanisms in the Unsaturated Zone at Yucca Mountain: From Pore-scale Physics to an Improved Understanding of Drift- and Large-scale Flow Processes - J.T. Birkholzer et al.

Feature and Fault Testing & Analysis

- **Determine in-block fault channeling and interface diversion capacities with liquid tracer testing**
- **Evaluate redistribution of percolation flux at features and faults with associated modeling**
- **In-plane borehole testing and monitoring to quantify near-drift alterations and away-from-drift conditions**







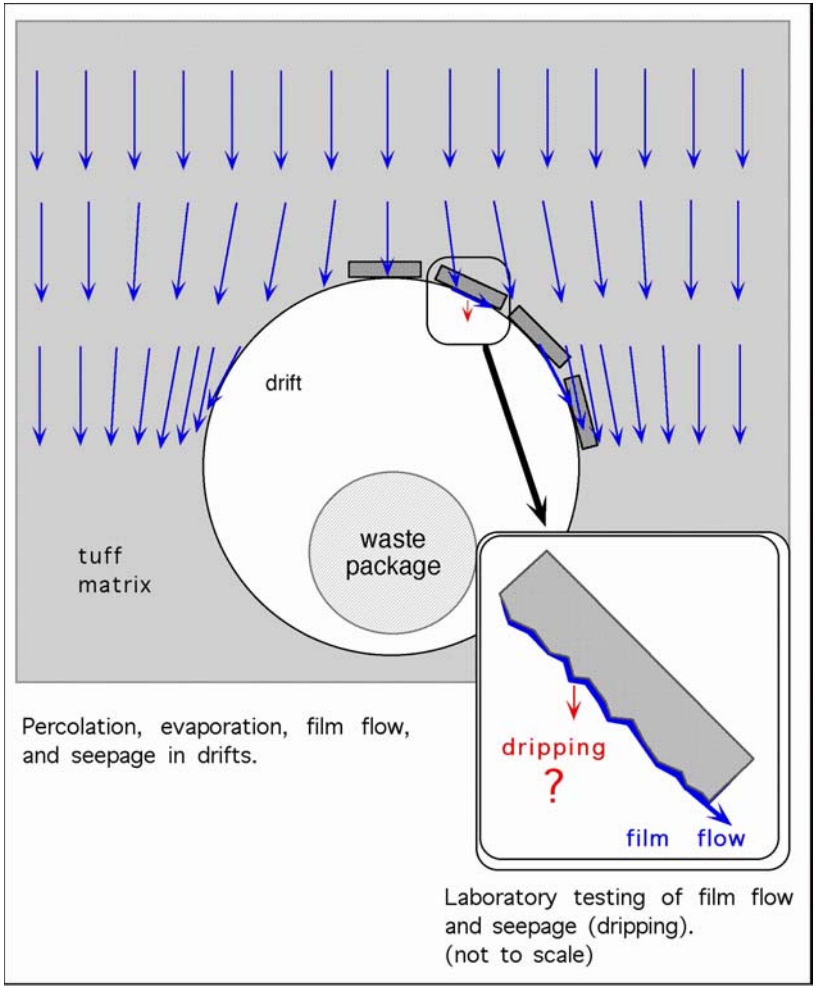
Feature and Fault Testing and Analysis - J.S. Wang et al.

Focus Areas

- UZ Flow
- Man-Made Natural Barriers: Evaluate (E) Film Flow and Seepage, (F) Near-Drift Moisture Dynamics, (G) Ventilation, and (H) Drift Shadow
- UZ Transport
- Coupled Processes
- Volcanism
- Natural Analogues / International Collaboration

Film Flow Reduces Seepage onto Waste Packages

- **Quantify film flow along drift walls as a mechanism for water bypassing WP's**
- **Estimate wall roughness and drift degradation in altering the partition between film flow and seepage**
- **Model flow field changes due to fracture dilation, rock fall, and cavities**



Capillary Barrier Effects, Film Flow, and Seepage from Drift Walls - T.K. Tokunaga et al.

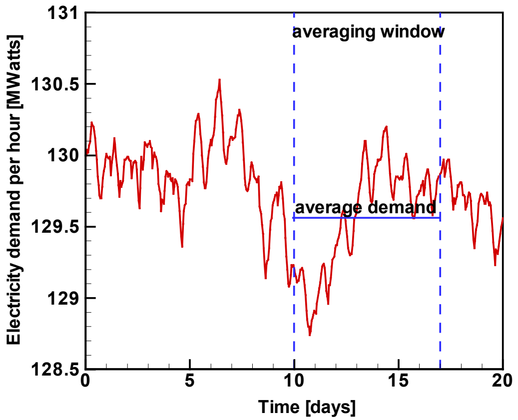
In-Drift Moisture Dynamics

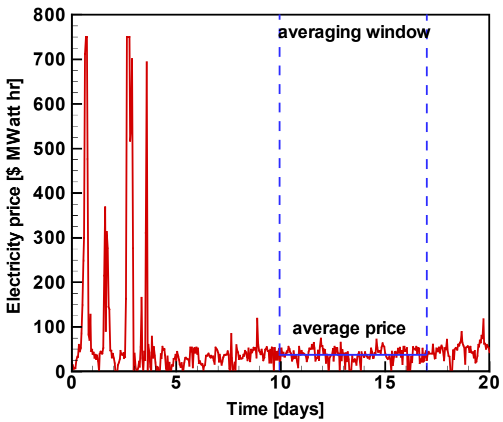
- **Evaluate observed water driven by thermal gradient or seepage inflow in sealed drift segments behind bulkheads**
- **Quantify temperature and moisture heterogeneity along drifts and boreholes in high infiltration areas**
- **Assess chemical and biological changes on metal and rock surfaces by monitoring and modeling**

Experimental and Modeling Study of Near-Drift Moisture Dynamics - R. Salve et al.

Optimization of Ventilation and Thermal Loading

- **Forced ventilation to keep drift wall temperatures below regulatory limit can be costly (e.g. 35 M / year)**
- **Use decision-management framework with numerical model to forecast electricity demand of ventilation system; financial based real option model to value alternative ways of purchasing electricity**

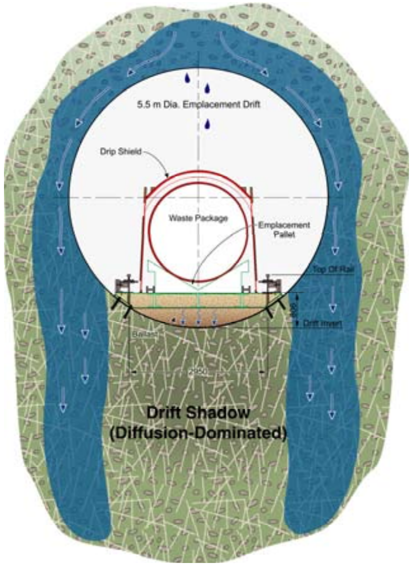


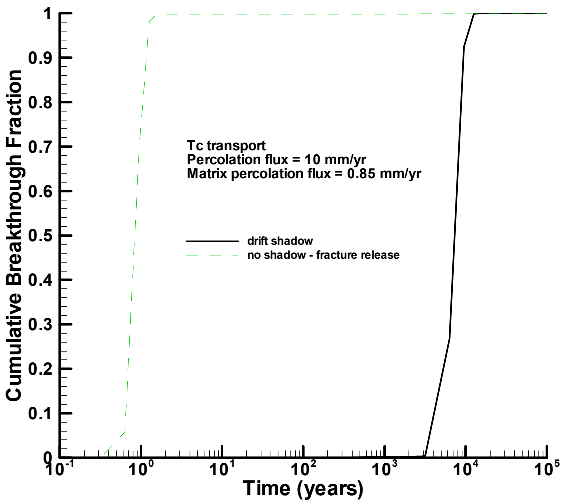


A Decision-Management Framework for the Design and Operation of the Preclosure Ventilation System for Thermal Load Control - A. Unger et al.

Drift Shadow Impacts

- **Matrix release concept adopted by TSPA (in SSPA) must be validated by ESF testing and natural analogue studies**
- **Effects of shadow in TSPA-SSPA show ~10,000 yr delay in dose**
- **Evaluate effects of rock heterogeneity and waste heat**





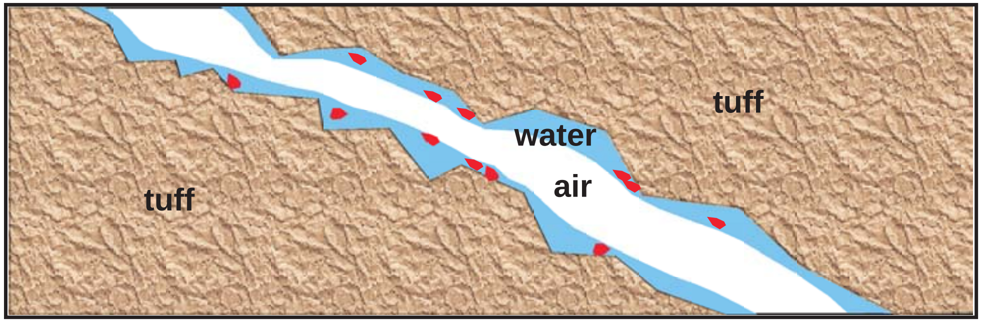
Evaluation of the Drift Shadow Model and Model Extensions - J.E. Houseworth et al.

Focus Areas

- UZ Flow
- Man-Made Natural Barriers
- UZ Transport: Evaluate (I) Colloid and Nanoparticle Transport, (J) Diffusion and Sorption in Fractured Blocks, and (K) Spatial Discretization
- Coupled Processes
- Volcanism
- Natural Analogues / International Collaboration

Colloid and Nanoparticle Transport in Rock and Fractures

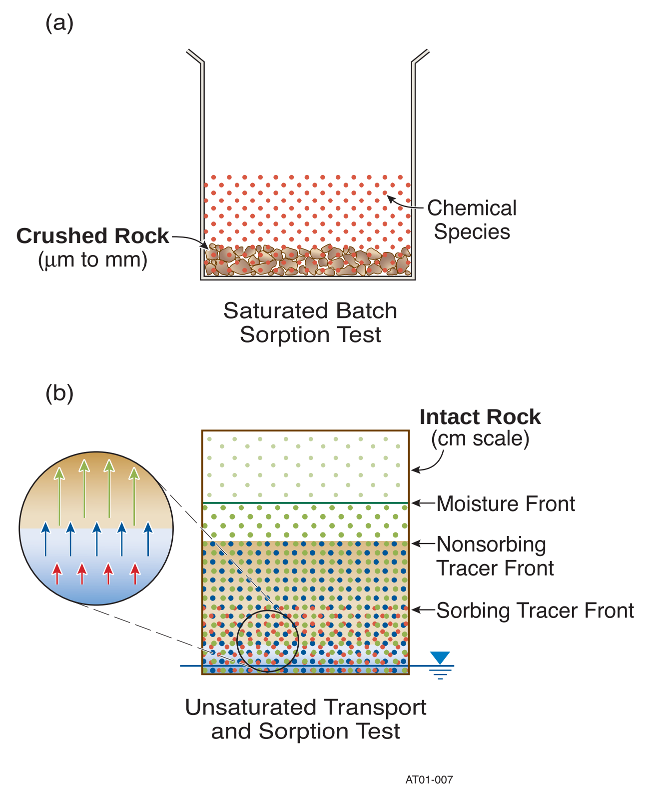
- Evaluate colloid migration (and filtration) into small- pore matrix and dry fractures in the shadow zone
- Determine the relative importance of nanoparticles to transport
- Provide experimentally tested, site-specific data for conceptual and predictive model for colloid transport in UZ



Colloid and Nanoparticle Transport in YM Rock and Fractures - J. Wan et al.

Diffusion and Sorption on UZ Radionuclide Transport

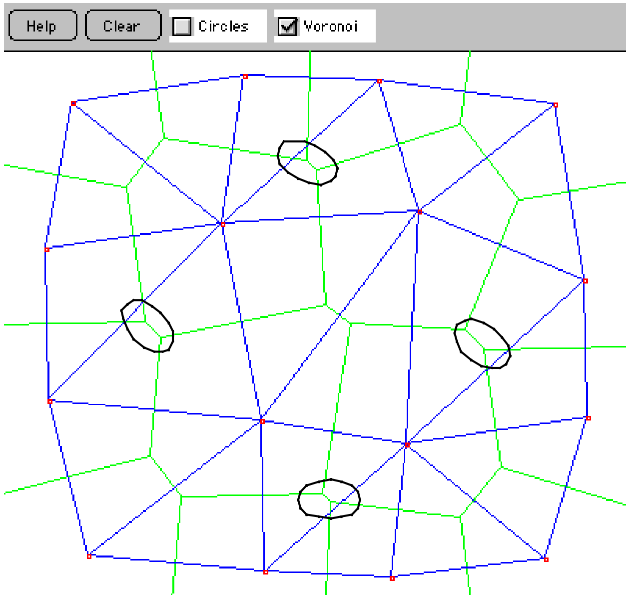
- **Reduce uncertainties associated with using batch saturated sorption experiments with crushed samples**
- **Conduct in-tact core and cubic meter block tests to quantify diffusion, fracture-matrix interaction, and effects of fracture-network heterogeneity on matrix diffusion/sorption**



Effects of Diffusion and Sorption on Radionuclide Transport in the UZ of YM - Q. Hu et al.

Developing Appropriate Spatial Discretization

- Minimize errors of inappropriately designed numerical grids in models that could impact TSPA
- Develop methodology for generating multi-nodal connected 3-D grids
  - define new geometries in TOUGH2
  - apply new gridding method to problems entailing sloping layers, fault offset, pinchout, and local refinement needed for 3-D models



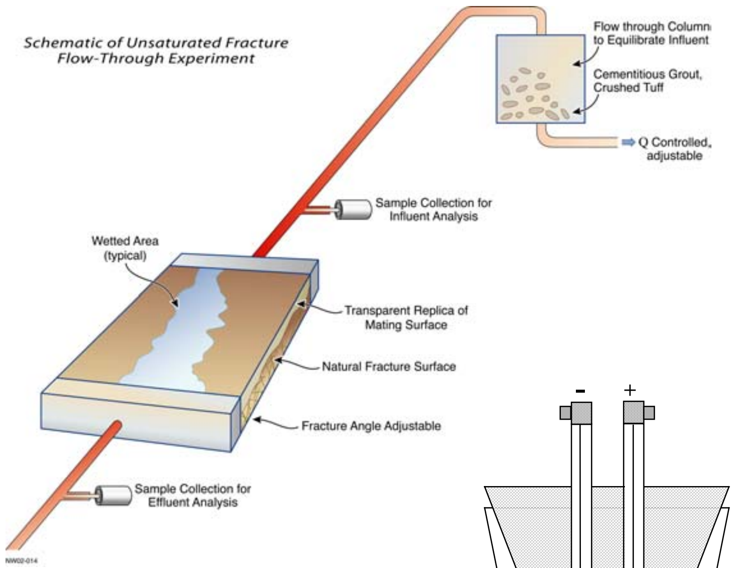
Developing Appropriate Spatial Discretization for 3-D UZ Flow and Transport Models - K. Pruess

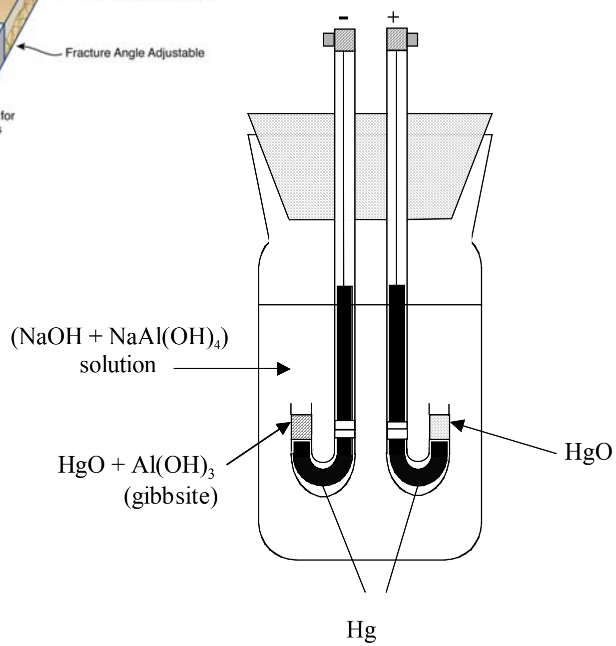
Focus Areas

- UZ Flow
- Man-Made Natural Barriers
- UZ Transport
- Coupled Processes: (L) Reactive Transport, (M) THC and THM Induced Changes, and (O) Cross Drift Thermal Test in Lower Lithophysal Tuff
- Volcanism
- Natural Analogues / International Collaboration

THC Reactive Transport Parameters and Processes

- **Evaluate reaction rates of coating minerals in natural fractures which controls water chemistry - important for WP corrosion rates (especially high ionic strength fluids)**
- **Quantify relation between wetted surface area, saturation, and reaction rates in natural fractures - fracture permeability changes that control seepage rates**

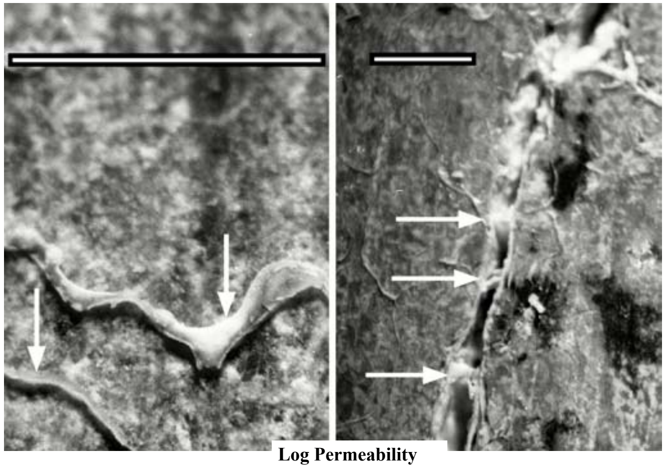


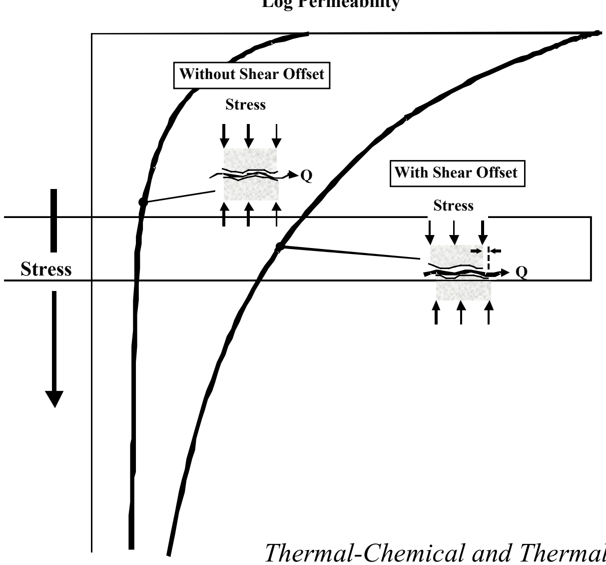


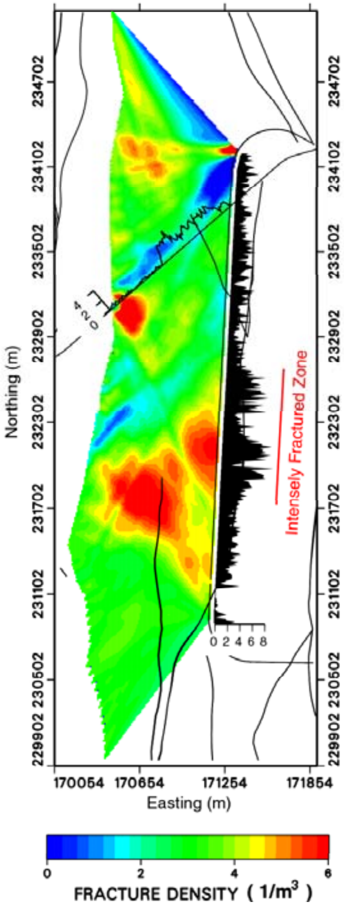
Laboratory and Modeling Investigation into Reactive Transport Parameters and Processes in the UZ - E.L. Sonnenthal et al.

THC & THM Effects on Fracture and Matrix Properties

- **Quantify permeability alteration near drifts caused by drift mining and heating (damage zone)**
- **Reduce uncertainties in predictions of flow around drifts and seepage caused by THC and THM effects:**
  - **stress-k relationship**
  - **chemical precipitation**
  - **Water properties on imbibition**



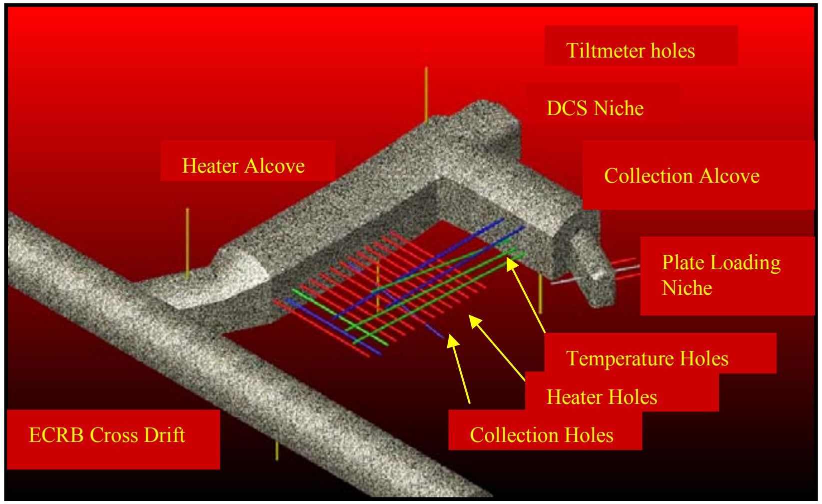




Thermal-Chemical and Thermal-Mechanical Effects on Fracture and Matrix Properties - T.J. Kneafsey et al.

Cross-Drift Thermal Test

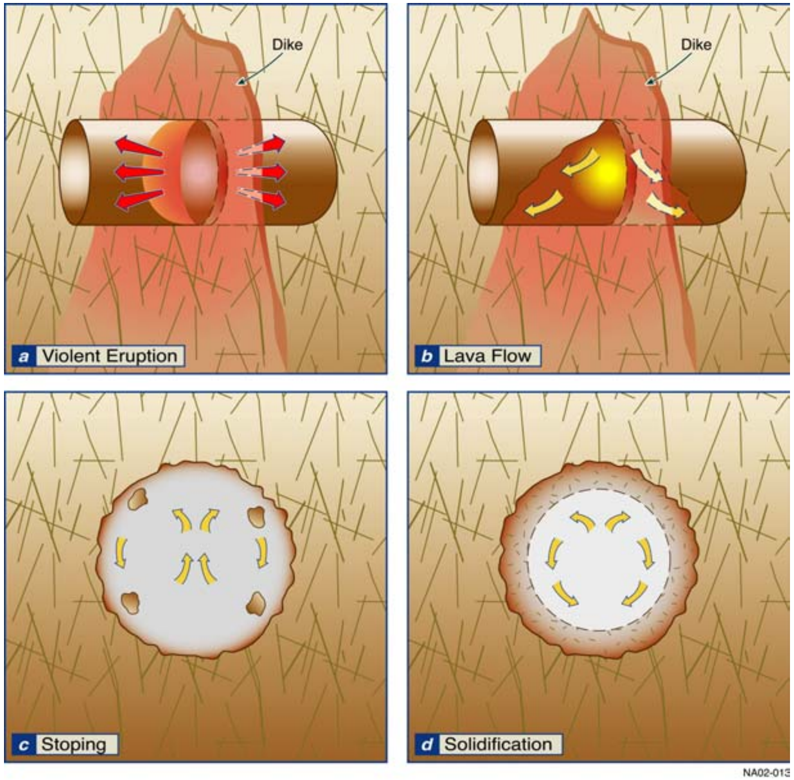
- **70% of potential repository will be in lower lithophysal unit - Need CDTT for uncertainty reduction**
- **Determine impact of lithophyscal cavities on THMC processes; test seepage water and gas chemistry; test drainage between drifts; test absence of water penetration through hot zone; analyze THC with sufficient mobilized water**



The Cross-Drift Thermal Test - Y.Tsang and S. Mukhopadhyay

Volcanism Consequence - Magma Intrusion into Drifts

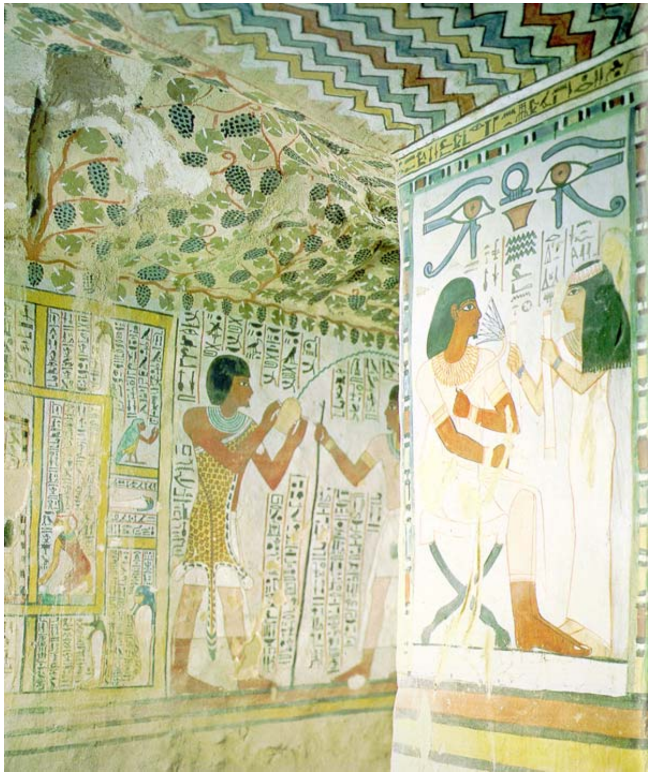
- Understand thermal, mechanical and moisture effects associated with magma intrusion into drifts
- Evaluate effects of magma intrusion in affecting flow and transport in UZ



Multiscale Thermomechanical Effects of Magma Intrusion on Drifts and the Unsaturated Zone - C.M. Oldenburg et al.

Natural Analogues

- **To build confidence in public and scientific community**
  - **- Peña Blanca**
  - **- Bangombé**
  - **- Rainier Mesa**
  - **- Man-made Materials**
  - **- Microbes**
  - **- Drift Shadow**
  - **- Other Transport**



Natural Analogues - A.M. Simmons et al.

International Collaboration

- **International Center**
- **Coupled processes - Febex, DECOVALEX, thermochemical database**
- **Transport - Äspö, deep injection sites Russia, uranium mines Russia and China, colloids at Grimsel**
- **Transportation**

International Collaboration - A.M. Simmons et al.

Summary

- Cost reduction can be achieved by evaluating natural barriers to reduce uncertainties and collect data for realistic representation of Yucca Mountain
- Proposals are prepared to address key scientific issues:
  - ∗ UZ Flow - greenhouse climate, geochemistry, focusing, fault
  - ∗ Man-Made Natural Barriers - film flow, in-drift moisture, ventilation, drift shadow
  - ∗ UZ Transport - colloid, cubic meter block, grid
  - ∗ Coupled Processes - reactive transport, THC/THM, CDTT
  - ∗ Volcanism - consequence of magma invasion on UZ
  - ∗ Natural Analogues / International Collaboration

Concluding Remark

- While most of the UZ barrier capacities are recognized since SCP development and ESF excavation, many new and advance scientific and technological issues are identified not only for uncertainty reduction and realistic representation, but more importantly for fundamental knowledge about features, events, and processes in this unique desert setting with deep UZ. Excitement in new discoveries is best for establishing conviction that the Yucca Mountain site is suitable for safe disposal over long times.